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Quantum transport equations for high electric fields

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We have studied quantum-mechanical transport equations for nondegenerate electrons in semiconductors in high electric fields. Our calculations use Kadanoff and Baym's formalism based on Green functions, treat only fields that are constant in space and time, and are restricted to weak scattering. First, we derive an approximate solution to the equation of motion of the retarded Green function in an electric field, with a careful check of its validity. This is used in deducing the conditions under which the quantum-mechanical transport equation reduces to the Boltzmann equation. We find, in agreement with some previous studies, that the electric field causes a "broadening" of the δ function in semiclassical transition rates, a result of the "intracollisional field effect." The Boltzmann equation fails when this broadening exceeds some characteristic energy scale (usually $k_B T$), which occurs at fields of a few MV m^{-1} in conventional semiconductors. These results are strongly dependent on the *ansatz* used to reduce the Green function to a distribution function. The scattering-out term is usually much less sensitive to the electric field than the scattering-in term. We exploit this to construct an integral transport equation, valid in high electric fields, which differs from the Boltzmann equation only in having a broadened function replacing the δ function in the scattering-in rates. It should be possible to solve this equation using standard numerical techniques and gain quantitative information on the intracollisional field effect.

I. INTRODUCTION

The theory of transport in semiconductors has traditionally been based on the semiclassical Boltzmann equation,[1-3] but the modeling of devices currently under development is pushing this equation to its limits.[4] The size of modern devices is shrinking continually while applied voltages remain about the same, which means that the typical electric fields are becoming very large and rapidly varying in space. Does the Boltzmann equation remain valid under such extreme conditions?

For example, recent experiments[5,6] have demonstrated directly the existence of ballistic carriers in semiconducting devices, signifying a distribution function nowhere near its thermal form. Important features of these experiments are the following: high electric fields (exceeding 10^6 V m^{-1}), which accelerate the ballistic electrons and drive the distribution far from equilibrium; contact effects, which are used to inject the electrons over a barrier[5] or through a tunnel junction,[6] and which rely on rapid spatial variation of the electric field to launch the ballistic carriers; and very high scattering rates, which necessitate an extremely narrow active region (30–60 nm) to preserve the ballistic features.

Solutions of the Boltzmann equation in submicrometer devices[7-11] have already revealed striking ballistic structure in the distribution function. However, these experiments emphasize important basic questions concerning the validity of the Boltzmann equation.

(i) Can transition rates calculated using the golden rule be used even in the presence of a high (uniform) electric field as, for example, in Refs. 5 and 11?

(ii) At what strengths of electric field does the structure of the Boltzmann transport equation itself fail?

(iii) Do the electric field and density of electrons vary too rapidly in space for the semiclassical description to be applicable?

Our aim in this paper is to address the first two questions for the simplest situation, electrons in a parabolic band accelerated by a uniform electric field and scattered weakly by phonons. This paves the way for an approach to the more complicated problem of inhomogeneous systems, strong scattering, and the modeling of real semiconductor devices.

The Boltzmann equation for a nondegenerate system in a uniform electric field $\mathbf{F}(t)$ can be written

$$\left[\frac{\partial}{\partial t}+e\mathbf{F}(t)\cdot\nabla_k\right]f_{\rm cl}(\mathbf{k},t)=\sum_{\mathbf{q}}[W(\mathbf{k},\mathbf{k}-\mathbf{q})f_{\rm cl}(\mathbf{k}-\mathbf{q},t) - W(\mathbf{k}+\mathbf{q},\mathbf{k})f_{\rm cl}(\mathbf{k},t)]\ , \quad (1.1)$$

where $f_{\rm cl}$ is the semiclassical distribution function. The second term on the right-hand side (RHS) can also be written as $-\Gamma(\mathbf{k})f_{\rm cl}(\mathbf{k},t)$ where

$$\Gamma(\mathbf{k})=\sum_{\mathbf{q}}W(\mathbf{k}+\mathbf{q},\mathbf{k}) \quad (1.2)$$

is the total scattering-out rate. An assumption in conven-

tional derivations of the Boltzmann equation is that collisions are instantaneous in time.[12] This has two important consequences for the collision term on the RHS of (1.1): it depends on $f_{\rm cl}$ only at time t, and not at times in the past; and the driving field $\mathbf{F}(t)$ does not appear. Neither of these simplifying features is true of the more rigorous quantum-mechanical transport equation, and essentially our task is to determine under what conditions the local collision term in (1.1) is accurate. We find a differential transport equation that agrees with Barker and Ferry,[13] and confirm their result that the Boltzmann equation fails in electric fields exceeding about 10^6–10^7 $\mathrm{V\,m^{-1}}$. We have also derived a new integral equation for describing transport in high electric fields. It differs from the Boltzmann equation only in having a "broadened" function replacing the δ function of the semiclassical scattering-in rates. It should be possible to solve this integral equation by the standard numerical techniques, because it has the simple scattering-out term of the Boltzmann equation with no extra integrations.

We treat electrons in a single band with dispersion relation $\varepsilon(\mathbf{k})$, which we shall ultimately take to be parabolic [$\varepsilon(\mathbf{k})=k^2/2m$, with m the effective mass]. The Hamiltonian including an applied field, which may enter through scalar and vector potentials, but excluding scattering, is

$$H_U(\mathbf{r},t)=\varepsilon(-i\nabla_r-e\,\mathbf{A}(\mathbf{r},t))+e\phi(\mathbf{r},t) \tag{1.3}$$

in units where $\hbar=1$; e is the charge on the carriers. Many important features of real devices and materials are absent from our model: more realistic band-structure permitting interband transitions, spatially varying electric fields, and polaronic effects for example. We feel that it is better first to understand a simple model properly, to provide a firm foundation for exploring more complicated systems and processes. Even this simple model has led to much controversy, with widely differing estimates for the maximum field in which the Boltzmann equation is valid.[13–16]

Our calculations use the nonequilibrium Green functions introduced independently by Kadanoff and Baym[17] and by Keldysh.[18] We provide a brief review of these techniques in Sec. II. Two vital features of the calculation are a redefinition of the variables to ensure gauge invariance, and the use of "reduced functions;" these have the spectral function in the presence of the field (but without scattering) factored out, removing much of the field dependence from their equations of motion. In Sec. III we derive an approximate solution for the retarded Green function, with a careful check of its accuracy. The kinetic equation is treated in Sec. IV. An *ansatz* is needed to reduce the equation involving Green functions to one for the distribution function. Our results, in particular the conditions under which the transport equation reduces to the Boltzmann equation, are very sensitive to the choice of this. An improved *ansatz,* recently introduced by Lipavsky *et al.*,[19] is vital to avoid losing the intracollisional field effect and to maintain symmetry between the scattering rates appearing in the different Green functions.

Appendix A contains a description of the numerical calculations used to verify the accuracy of the retarded Green function. Our conditions for the Boltzmann equation to be valid involve defining a "collision duration time;" in Appendix B we compare this with the "delay time" defined in scattering theory. We found it convenient to work with an integral transport equation rather than the more usual differential one, but we show in Appendix C that the latter leads to the same conclusions. Finally, in Appendix D, we consider a simple picture of the intracollisional field effect, and discuss how one might attempt to calculate transition rates from the golden rule, even in high electric fields.

II. QUANTUM TRANSPORT FORMALISM

In this section we shall briefly review and set up the equations for the nonequilibrium Green functions on which our calculations are based.

A. Introduction

The semiclassical theory of transport in semiconductors rests on the Boltzmann equation, whose differential form was given above [Eq. (1.1)]. $W(\mathbf{k}+\mathbf{q},\mathbf{k})$ is the transition rate from $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ given by the golden rule. For scattering from phonons,

$$W(\mathbf{k}+\mathbf{q},\mathbf{k})=2\pi\,|\,M_{\mathbf{q}}\,|^2\{(N_{\mathbf{q}}+1)\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\Omega_{\mathbf{q}})+N_{\mathbf{q}}\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})-\Omega_{\mathbf{q}})\} \tag{2.1}$$

$$\equiv 2\pi\,|\,M_{\mathbf{q}}\,|^2\sum_{\eta=\pm1}[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\eta\Omega_{\mathbf{q}})\,, \tag{2.2}$$

where $M_{\mathbf{q}}$ is the matrix element for scattering, $\Omega_{\mathbf{q}}$ is the frequency of the phonon, and $N_{\mathbf{q}}$ is the occupation number. The first term ($\eta=+1$) is for the emission of a phonon and the second ($\eta=-1$) for absorption. Umklapp processes do not appear because we are considering a single unbounded parabolic band. The Boltzmann equation (1.1) can also be written in an integral form. For a uniform, constant field this becomes

$$f_{\rm cl}(\mathbf{k})=\int_0^\infty dt\,\exp\left[-\int_0^t dt'\Gamma(\mathbf{k}-e\mathbf{F}t')\right]\times\sum_{\mathbf{q}}W(\mathbf{k}-e\mathbf{F}t,\mathbf{k}-\mathbf{q}-e\mathbf{F}t)f_{\rm cl}(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)\,, \tag{2.3}$$

where $\mathbf{k}-e\mathbf{F}t$ gives the evolution of a $\mathbf{k}$ vector with time according to $\dot{\mathbf{k}}=e\mathbf{F}$. The two formulas (1.1) and (2.3)

can readily be shown to be equivalent by operating on (2.3) with $e\mathbf{F}\cdot\nabla_k$ (this is made easier if the variables of integration t and t' are first replaced by the components of $\mathbf{k}-e\mathbf{F}t$ and $\mathbf{k}-e\mathbf{F}t'$ parallel to $\mathbf{F}$). A fuller proof is given in (for example) Ref. 3. The integral equation has the important feature that it can be solved numerically using iterative or Monte-Carlo techniques.

The interpretation of Eqs. (1.1) and (2.3) is simple. In the differential form (1.1), the RHS has the form "scattering-in"–"scattering-out." In the integral form (2.3), the sum involving $f_{\rm cl}$ gives the rate at which particles were scattered into $\mathbf{k}-e\mathbf{F}t$ a time t ago, and the exponential term gives the probability that such particles survive to the present with wave vector $\mathbf{k}$. The simplicity of these equations is due to the local nature of the collision term. This is not true of the quantum transport equations, as we shall see in the next sections.

The fully quantum-mechanical analog of the semiclassical distribution function $f_{\rm cl}$ is the Wigner function f, a Fourier transform of the density matrix:

$$f(\mathbf{k},\mathbf{R},T)=\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\rho(\mathbf{R}+\tfrac{1}{2}\mathbf{r},\mathbf{R}-\tfrac{1}{2}\mathbf{r},T)\ . \tag{2.4}$$

It is important here that f be expressed in terms of mechanical (or kinematical) momentum $\mathbf{k}$, *not* canonical momentum $\mathbf{p}$, in the presence of an applied field. This has been emphasized particularly by Levinson,[20] and we shall return to this point later.

We now need to set up a kinetic equation for f, valid in high electric fields. One of our aims in this paper is to determine the conditions under which this reduces to the Boltzmann equation. In linear-response theory, the fluctuation-dissipation theorem allows one to calculate transport coefficients from correlation functions of the ground state, i.e., in the absence of the applied field; thus conventional equilibrium perturbation theory can be used. We are interested in high electric fields, in which case the system may be driven far from equilibrium, well beyond the region of linear response. We are therefore obliged to use the more cumbersome apparatus of nonequilibrium statistical mechanics, and must include the applied field in that part of the Hamiltonian which is treated exactly. Approximations should be made only in the treatment of the scattering (phonons, impurities, etc.), and not in the strength of the applied field.

One route to a kinetic equation is to use the Liouville equation for ρ directly; this has been taken by Levinson,[20] Barker[21] and others. A second approach, which we follow here, is based on Green functions and was introduced by Kadanoff and Baym[17] and by Keldysh.[18] An elegant fusion of these two slightly different formalisms has been given by Langreth.[22] We give a summary of his results in the next section, following the notation of Jauho and Wilkins.[23]

B. Nonequilibrium Green functions

Rather than dealing with the density matrix directly, this formalism[22] is based on double-time correlation functions:

$$G^{<}(1,2)\equiv G^{<}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=i\langle\Psi_H^{\dagger}(2)\Psi_H(1)\rangle\ , \tag{2.5a}$$

$$G^{>}(1,2)\equiv G^{>}(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=-i\langle\Psi_H(1)\Psi_H^{\dagger}(2)\rangle\ . \tag{2.5b}$$

Langreth[22] explains the meaning of the nonequilibrium expectation values. Now we introduce sum and difference coordinates,

$$\begin{aligned}&\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2,\quad t=t_1-t_2\ ,\\ &\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2),\quad T=\tfrac{1}{2}(t_1+t_2)\ .\end{aligned} \tag{2.6}$$

Using these coordinates, the density matrix and Wigner function are given by

$$\rho(\mathbf{r},\mathbf{R},T)=-iG^{<}(\mathbf{r},t=0;\mathbf{R},T)\ , \tag{2.7a}$$

$$f(\mathbf{k},\mathbf{R},T)=\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\rho(\mathbf{r},\mathbf{R},T) \tag{2.7b}$$

so quantities of physical interest can be derived from $G^{<}(t=0)$.

Also important in the calculations are the retarded and advanced Green functions, which are defined conventionally, for example,

$$G^{r}(1,2)=-i\Theta(t_1-t_2)\langle\{\Psi_H(1),\Psi_H^{\dagger}(2)\}\rangle\ . \tag{2.8}$$

It is important to note that the distribution function *cannot* be obtained from $G^{r,a}$; essentially they describe the propagation of an extra particle added to the system. The Green functions are interconnected by the spectral function A:

$$A=i[G^{r}-G^{a}]=i[G^{>}-G^{<}]=\langle\{\Psi_H(1),\Psi_H^{\dagger}(2)\}\rangle\ , \tag{2.9}$$

A obeys a sum rule at $t_1=t_2$ which follows from the anticommutation relation of the operators in (2.9). It is important to note that G^{r}, G^{a}, and A contain the same information, for example,

$$G^{r}(t_1,t_2)=-i\Theta(t_1-t_2)A(t_1,t_2)\ , \tag{2.10}$$

but knowing A alone is *not* enough to determine $G^{<}$ or $G^{>}$ except in thermal equilibrium. Define the Fourier transform by

$$G^{<}(\mathbf{p},E;\mathbf{R},T)=\int d\mathbf{r}\int dt\, e^{-i(\mathbf{p}\cdot\mathbf{r}-Et)}G^{<}(\mathbf{r},t;\mathbf{R},T)\ . \tag{2.11}$$

In equilibrium there can be no dependence on T, and $G^{<}$ and $G^{>}$ obey

$$G^{<}(\mathbf{p},E;\mathbf{R})=iA(\mathbf{p},E;\mathbf{R})f_{\rm FD}(E)\ , \tag{2.12a}$$

$$G^{>}(\mathbf{p},E;\mathbf{R})=-iA(\mathbf{p},E;\mathbf{R})[1-f_{\rm FD}(E)]\ , \tag{2.12b}$$

where $f_{\rm FD}(E)$ is the Fermi-Dirac distribution function.[17] No such relation holds away from equilibrium, and separate equations are then needed to find $G^{r,a}$ and $G^{<,>}$. In Langreth's lucid paper these are derived from a Green function ordered on a generalized contour in complex time, rather than from $-\infty$ to ∞ or from 0 to $-i\beta$ as in the usual formalism restricted to systems at zero temperature or in thermal equilibrium. The retarded and advanced Green functions satisfy the familiar Dyson equations, written symbolically as

$$G^{r}=G_0^{r}+G_0^{r}\Sigma^{r}G^{r}=G_0^{r}+G^{r}\Sigma^{r}G_0^{r}\ . \tag{2.13}$$

The self-energy Σ^r is in general a functional of $G^{<,>}$ as well as $G^{r,a}$. We aim to make no approximation in the strength of the applied field, as emphasized in Sec. II A. To achieve this, we take G_0 to be the Green function for an electron in the presence of the applied field but without scattering, corresponding to the Hamiltonian H_U [Eq. (1.3)], and denote it by G_U as a reminder of this.

Because $G^<$ contains the distribution function as a limiting case, its equation of motion is analogous to the classical kinetic equation. Like the Boltzmann equation, this can be written in "differential" (strictly, integro-differential) and "integral" forms.

The differential equation of motion for $G^<(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ with $t_1=t_2=T$ can be written symbolically as[23]

$$-[G_U^{-1},G^<]=\int_{-\infty}^{T}dt'\int d\mathbf{r}'[\{\Sigma^<,G^>\}-\{\Sigma^>,G^<\}]\ , \tag{2.14}$$

where the operator G_U^{-1} is defined (as usual) as

$$G_U^{-1}(\mathbf{r},t)=i\frac{\partial}{\partial t}-H_U(\mathbf{r},t)\ , \tag{2.15}$$

and $\Sigma^{<,>}$ are self-energies or scattering rates which will be considered in more detail in Sec. II D. As usual, the self-energies are themselves functionals of the Green functions. Equation (2.14) can be directly compared with the Boltzmann equation, which is an attractive feature of the formalism. The left-hand side (lhs) reduces to exactly the same form in a uniform applied field. $G^<$ is a "density of particles" and $\Sigma^>$ can be interpreted as a scattering-out rate, so that the anticommutator $\{\Sigma^>,G^<\}$ corresponds precisely to the scattering-out term of the Boltzmann equation; likewise the other term represents scattering in.

An important difference from Boltzmann theory is the presence of the integrals in the collision term: it is explicitly retarded in time and nonlocal in space. This means that the driving forces appear within the collision term, as well as on the left-hand side, giving rise to "intracollisional field effects." Also apparent is a serious difficulty inherent in this method: we want $G^<(\mathbf{r},t;\mathbf{R},T)$ only for $t=0$ to derive physical quantities, but need it for all t to perform the integral over time in the collision term. The usual way around this problem is to make an *ansatz* for the dependence of $G^<$ on t; we shall return to this important point in Sec. II E.

The integral equation[24] can be written as

$$G^<(1,2)=\int d1'\int d2'G^r(1,1')\Sigma^<(1',2')G^a(2',2)\ . \tag{2.16a}$$

$\Sigma^<(1',2')$ gives the rate at which particles are scattered "in," $G^r(1,1')$ gives the probability amplitude that they survive from 1' to 1 without being scattered "out," and $G^a(2',2)$ "completes the square" to give a probability density. We have dropped from this equation a boundary term,[25]

$$\int d\mathbf{r}_1'\int d\mathbf{r}_2'G^r(1;\mathbf{r}_1',t_0)G^<(\mathbf{r}_1',t_0;\mathbf{r}_2',t_0)G^a(\mathbf{r}_2',t_0;2)\ , \tag{2.16b}$$

which depends on t_0, the time at which the interaction with phonons was turned on. We assume that this happened in the distant past so that any influence of this term has decayed owing to the damping in G^r and G^a.

Note that the scattering-in and scattering-out terms enter the integral equation in a very asymmetric way, as they do in the integral form of the Boltzmann equation. This means that it is vital to follow the rules laid down by Kadanoff and Baym[17] for conserving approximations to ensure that the correct symmetry between the scattering rates is preserved. By contrast, the more symmetric basic structure of the differential equation allows greater liberties to be taken with approximations.

An attractive feature of Langreth's formalism is that the equations of motion for the single-particle properties $G^{r,a}$ [Eq. (2.13)] and those for the distribution properties $G^{<,>}$ [Eq. (2.14)] appear to be independent. This is not quite true, because the equation for $G^{r,a}$ depends implicitly on $G^{<,>}$ through the self-energy $\Sigma^{r,a}$, but for a nondegenerate system this dependence is negligible (Sec. II D) and the two sets of equations are decoupled. This permits a two-step procedure for solving the problem.[23] First, one solves the Dyson equation (2.13), which gives the retarded Green function (and spectral function). This provides information about the scattering of an extra particle added to the system. The spectral function is then used to construct an *ansatz* for $G^{<,>}$ (Sec. II E), which is in turn used to reduce the equation of motion for $G^<$, (2.14) or (2.16), to a transport equation for the distribution function.

In the main body of this paper we shall concentrate on the solution of the integral transport equation, because we have found that it is more straightforward to draw physical conclusions from this formalism. However, we show in Appendix C that the differential equation leads to identical results, although its interpretation is more tricky.

C. Field-dependent Green functions and reduced functions

It is most convenient to introduce a uniform electric field by a vector potential[26] because canonical momentum $\mathbf{p}$ is a conserved quantity in this gauge. Then G_U^r, the retarded Green function in the presence of the field, obeys the pair of equations

$$G_U^{-1}G_U^r\equiv\left[i\frac{\partial}{\partial t_1}-\varepsilon(\mathbf{p}-e\,\mathbf{A}(t_1))\right]G_U^r(\mathbf{p};t_1,t_2)$$
$$=\delta(t_1-t_2)\ , \tag{2.17a}$$

$$G_U^rG_U^{-1}\equiv\left[-i\frac{\partial}{\partial t_2}-\varepsilon(\mathbf{p}-e\,\mathbf{A}(t_2))\right]G_U^r(\mathbf{p};t_1,t_2)$$
$$=\delta(t_1-t_2)\ , \tag{2.17b}$$

with the boundary condition that $G_U^r(\mathbf{p};t_1,t_2)=0$ for $t_1<t_2$. The solution of these equations is trivial as they are first-order in time:

$$G_U^r(\mathbf{p};t_1,t_2)=-i\Theta(t_1-t_2)\times\exp\left[-i\int_{t_2}^{t_1}d\tau\,\varepsilon(\mathbf{p}-e\,\mathbf{A}(\tau))\right], \tag{2.18}$$

from which the spectral function is

$$A_U(\mathbf{p};t_1,t_2)=\exp\left[-i\int_{t_2}^{t_1}d\tau\,\varepsilon(\mathbf{p}-e\,\mathbf{A}(\tau))\right]. \tag{2.19}$$

An important feature of A_U is that it can be factored[24,27] into the form

$$A_U(\mathbf{p};t_1,t_2)=\exp[-i\alpha(\mathbf{p},t_1)]\exp[i\alpha(\mathbf{p},t_2)]\ . \tag{2.20}$$

This formula shows that A_U can be factored out of all the Green functions and self-energies in the equations of motion while they are written in terms of canonical momentum $\mathbf{p}$, with adjacent pairs of exponential factors cancelling. To exploit this, we define reduced functions[24,27] by

$$G(\mathbf{p};t_1,t_2)=A_U(\mathbf{p};t_1,t_2)g(\mathbf{p};t_1,t_2)\ , \tag{2.21}$$

where G can be any Green function or self-energy, and a lower-case letter denotes the corresponding reduced function. The advantage of these functions is that much of the field dependence has been removed; for example,

$$g_U^r(\mathbf{p};t_1,t_2)=-i\Theta(t_1-t_2),\quad a_U(\mathbf{p};t_1,t_2)=1\ . \tag{2.22}$$

The self-energies σ are also brought closer to their equilibrium forms by this transformation, as we shall see in Sec. II D. The Dyson equation (2.13) for G^r, written in terms of canonical momentum and converted to reduced functions, becomes

$$g^r(\mathbf{p};t_1,t_2)=g_U^r(\mathbf{p};t_1,t_2)+\int dt_1'\int dt_2' g_U^r(\mathbf{p};t_1,t_1')\sigma^r(\mathbf{p};t_1',t_2')g^r(\mathbf{p};t_2',t_2)\ , \tag{2.23}$$

and the integral transport equation (2.16a) likewise becomes

$$g^<(\mathbf{p};t_1,t_2)=\int dt_1'\int dt_2' g^r(\mathbf{p};t_1,t_1')\times\sigma^<(\mathbf{p};t_1',t_2')g^a(\mathbf{p};t_2',t_2)\ . \tag{2.24}$$

Note that when $t_1=t_2$, $A_U(\mathbf{p};t_1,t_2)=1$ (by the usual sum rule), so $G^<=g^<$.

The above equations cannot usually be solved exactly, and it is vital to bring them to a less gauge-dependent form before approximations are made. In the case of a uniform field this means that all functions should be expressed in terms of mechanical momentum $\mathbf{k}$ rather than canonical momentum $\mathbf{p}$. It can be shown[18,20,28] that this is sufficient to ensure that the Green functions and distribution function become gauge invariant and spatially invariant in uniform fields. The Green functions will not be gauge invariant in time-varying fields, but that is unimportant here. We carry this out by redefining all functions as follows:

$$g(\mathbf{p},t;T)=g[\mathbf{k}+e\,\mathbf{A}(T),t;T]=\tilde{g}(\mathbf{k},t;T)\ , \tag{2.25}$$

where

$$\mathbf{k}=\mathbf{p}-e\,\mathbf{A}(T)\ , \tag{2.26}$$

and sum and difference coordinates are used for the times. Only differences of vector potentials will appear in the equations after this transformation.

We shall now specialize to the case of a constant electric field, with $\mathbf{A}(T)=-\mathbf{F}T$, and assume that a steady state has been reached. In this case all "T" variables drop out as one would expect physically; this also relies on $\mathbf{p}$ having been replaced by $\mathbf{k}$. Using Eqs. (2.4), (2.7), (2.21), and (2.26), the kinetic equation (2.24) for $\tilde{g}^<(\mathbf{k},t=0)$ becomes

$$if(\mathbf{k})\equiv\tilde{g}^<(\mathbf{k},t=0)=\int dt_1\int dt_2\tilde{g}^r(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}t_1,t_1)\tilde{\sigma}^<(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}(t_1+t_2),t_2-t_1)\tilde{g}^a(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}t_2,-t_2)\ . \tag{2.27}$$

In the future we shall drop the tildes and all functions of sum and difference times should be assumed to be the "tilde" functions. It turns out to be more convenient to use the differential equation of motion for g^r than the integral Dyson equation (2.23). Applying the operator G_U^{-1} to both forms in (2.13) and adding them, we obtain symbolically

$$\tfrac{1}{2}\{G_U^{-1},G^r\}=1+\tfrac{1}{2}\{\Sigma^r,G^r\}\ . \tag{2.28}$$

Going to reduced functions, and replacing $\mathbf{p}$ with $\mathbf{k}$, this becomes

$$i\frac{\partial}{\partial t}g^r(\mathbf{k},t)=\delta(t)+\tfrac{1}{2}\int_{-\infty}^{\infty}d\tau\{g^r(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau,t-\tau)\sigma^r(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}(t-\tau),\tau)+\sigma^r g^r\}\ . \tag{2.29}$$

Only the range $0<\tau<t$ contributes to the integral, because of the Θ functions in $g^r(\mathbf{k},t)$ and $\sigma^r(\mathbf{k},t)$.

The spectral function (2.19), expressed in these new variables, becomes

$$A_U(\mathbf{k},t)=\exp\left[-i\int_{-t/2}^{t/2}d\tau\,\varepsilon(\mathbf{k}+e\mathbf{F}\tau)\right], \tag{2.30}$$

which takes the explicit form for a parabolic band

$$A_U(\mathbf{k},t)=\exp\left[-i\frac{1}{2m}[k^2t+\tfrac{1}{12}(eF)^2t^3]\right], \tag{2.31}$$

with Fourier transform

$$A_U(\mathbf{k},E)=2\pi\frac{1}{w}\mathrm{Ai}\left[-\frac{1}{w}[E-\varepsilon(\mathbf{k})]\right], \tag{2.32}$$

where the "width" $w=[(eF)^2/8m]^{1/3}$, and $\mathrm{Ai}(z)$ is the Airy integral function of the first kind (Ref. 29, p. 446). It is interesting that $A_U(\mathbf{k},E)$ depends only on $|\mathbf{k}|$ even though $\mathbf{F}$ has broken the spherical symmetry of the system. Note that $A_U(\mathbf{k},E)\to 2\pi\delta(E-\varepsilon(\mathbf{k}))$ as $F\to 0$ (in the absence of scattering). In a translationally invariant system with no applied field the spectral function is nonnegative (even with scattering included), but the field $\mathbf{F}$ breaks the symmetry and A may change sign, as it does here. The presence of the F^2t^3 term in $A_U(\mathbf{k},t)$ gives rise to the broadening in $A_U(\mathbf{k},E)$, but, as we shall see in the next section, many physical quantities involve products like $A_U(\mathbf{k}_1,t)A_U(\mathbf{k}_2,-t)$ and this term cancels. This means that using the spectral function for electrons in the *absence* of a field would have given the same result. It does not imply that the electric field leaves the transition rates, etc., unchanged, however, but means that the modifications occur through time dependence of momenta rather than through broadening of the spectral function *per se*.

D. Self-energies and scattering rates

We next need an expression for the self-energies. The scattering from phonons will be treated to lowest order (Born approximation) which means that only the diagram

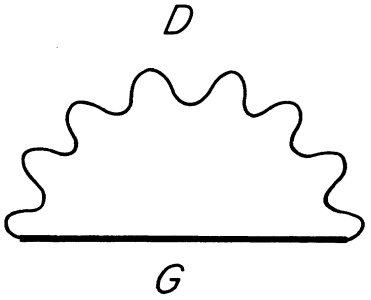

FIG. 1. Born approximation to the self-energy from electron-phonon scattering.

in Fig. 1 is included; D is the Green function for phonons including the matrix elements at the vertices. Note that we are dealing with a nondegenerate system, and cannot appeal to Migdal's theorem as justification for omitting higher-order diagrams.

This diagram is in the contour-ordered Green function. Langreth[22] has given rules for deriving the contribution to the functions $\Sigma^{<,>,r,a}$:

$$\Sigma^{<,>}(1,2)=iG^{<,>}(1,2)D^{<,>}(1,2), \tag{2.33a}$$

$$\Sigma^{r,a}(1,2)=i[G^{r,a}(1,2)D^{>}(1,2)+G^{<}(1,2)D^{r,a}(1,2)]. \tag{2.33b}$$

In a nondegenerate system, the low density of occupied states means that $G^<$ is small compared with $G^{r,a}$ and we therefore neglect the second term in (2.33b). This decouples $G^<$ from the equation of motion from G^r, an important simplification mentioned earlier. The expressions for the reduced functions (defined by $\Sigma=A_U\sigma$), assuming that the phonons always remain in equilibrium, are

$$\sigma^{<}(\mathbf{k},t)=\sum_{\substack{\mathbf{q}\\ \eta=\pm1}}|M_{\mathbf{q}}|^2[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]e^{i\eta\Omega_{\mathbf{q}}t}A_U^{-1}(\mathbf{k},t)A_U(\mathbf{k}-\mathbf{q},t)g^{<}(\mathbf{k}-\mathbf{q},t), \tag{2.34a}$$

$$\gamma(\mathbf{k},t)=\sum_{\substack{\mathbf{q}\\ \eta=\pm1}}|M_{\mathbf{q}}|^2[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]e^{-i\eta\Omega_{\mathbf{q}}t}A_U^{-1}(\mathbf{k},t)A_U(\mathbf{k}+\mathbf{q},t)a(\mathbf{k}+\mathbf{q},t), \tag{2.34b}$$

where we have introduced the reduced scattering rate $\gamma=i(\sigma^r-\sigma^a)=i(\sigma^>-\sigma^<)$, which is the spectral function for the reduced self-energy. In this equation, A^{-1} is just the reciprocal of the spectral function, not an operator.

To maintain a conserving approximation,[17] $g^<$ and a in the above expressions (2.34) should be derived from the self-consistent solution of (2.27), (2.29), and (2.34). In other words, scattering should be included *within* the Green function G used to calculate the self-energy in Fig. 1. In practice this is almost never done for γ when the scattering is weak, with the assumption that the scattering rates are not affected significantly by the small "blurring" of energy conservation introduced by the broadening in G. We shall follow the usual practice, and assume that the scattering is weak enough that we may set the reduced spectral function $a=1$ (i.e., replace A by A_U) to calculate γ. The validity of this will be considered in more detail in Sec. III B. The Fourier transform of (2.34b) is then given by

$$\gamma(\mathbf{k},\omega)=2\pi\sum_{\mathbf{q},\eta}|M_{\mathbf{q}}|^2[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\times\frac{1}{2\pi}\int_{-\infty}^{\infty}dr\exp\left[\left[\omega t-\eta\Omega_{\mathbf{q}}t+\int_{-t/2}^{t/2}d\tau[\varepsilon(\mathbf{k}+e\mathbf{F}\tau)-\varepsilon(\mathbf{k}+\mathbf{q}+e\mathbf{F}\tau)]\right]\right]. \tag{2.35}$$

A remarkable simplification, to which we alluded in the preceding section, now occurs for parabolic bands: all the terms in **F** drop out after the integration over τ, leaving

$$\gamma(\mathbf{k},\omega)=2\pi\sum_{\mathbf{q},\eta}|M_{\mathbf{q}}|^2[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)] \times\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\eta\Omega_{\mathbf{q}}-\omega) . \quad (2.36)$$

For $\omega=0$ this becomes the total semiclassical scattering-out rate $\Gamma(\mathbf{k})=\sum W(\mathbf{k}+\mathbf{q},\mathbf{k})$, a sum over scattering rates exactly as given by the golden rule in equilibrium [Eqs. (1.2) and (2.1)], but no approximation has been made in the strength of the electric field. Unfortunately, this result is amusing rather than useful, because the equation of motion (2.29) for g^r still contains the electric field in the time evolution of momenta; there is no simple factorization as in equilibrium. The analysis of this equation in Sec. III shows that $\gamma(\mathbf{k},\omega)$ is not an appropriate scattering rate to use, and new functions $\gamma_{\pm}(\mathbf{k},\omega)$ are introduced there which do not reduce to the simple form of Eq. (2.36)

E. Der Ansatz

A severe difficulty with this formalism, mentioned in Sec. II B, is that we only want to calculate $\rho(T)=G^<(t=0;T)$ to derive physical quantities, but need $G^<$ for all values of t to solve the kinetic equation. The conventional way to circumvent this problem is to make an *ansatz* that expresses $G^<(t;T)$ in terms of $G^<(t=0;T)$ which we "know" because it is just the distribution function.

The usual argument starts from the exact result for uniform systems in thermal equilibrium [Eq. (2.12a)],

$$G^<(\mathbf{k},E)=iA(\mathbf{k},E)f_{\rm FD}(E) , \quad (2.37)$$

there is no dependence on T in equilibrium. If the system can be described well in terms of quasiparticles, $A(\mathbf{k},E)$ is strongly peaked near $E=\varepsilon(\mathbf{k})$. The width of the peak is $\tau_{\rm sc}^{-1}$, the inverse of the mean free time (scattering time). If this width is much less than k_BT, the energy scale on which $f_{\rm FD}(E)$ varies, the argument of $f_{\rm FD}$ may be replaced by $\varepsilon(\mathbf{k})$. This allows us to write[17]

$$G^<(\mathbf{k},E)\approx iA(\mathbf{k},E)f(\mathbf{k}) \quad (2.38)$$

which is a well-controlled approximation if

$$\tau_{\rm sc}^{-1}\ll k_BT . \quad (2.39)$$

This has been generalized in a straightforward way to nonequilibrium systems:[23]

$$G^<(\mathbf{k},E;T)\approx iA(\mathbf{k},E;T)f(\mathbf{k},T) \quad (2.40a)$$

or, making a Fourier transform,

$$G^<(\mathbf{k},t;T)\approx iA(\mathbf{k},t;T)f(\mathbf{k},T) . \quad (2.40b)$$

The two vital simplifications accomplished by this *ansatz* are the following: (a) the dependence of $G^<$ on t (or E) is now given entirely by the spectral function; (b) the distribution function appearing in the *ansatz* is now the Wigner function (or density matrix), which is conventional for transport equations, rather than one involving energies as in (2.37). This illustrates the two-step procedure for deriving transport equations mentioned earlier. Solving for G^r gives the spectral function A, which is then used with an *ansatz* to reduce the equation of motion for $G^<$ to a transport equation in terms of $f(\mathbf{k},\mathbf{R},T)$. Equation (2.40) clearly satisfies the exact result $G^<(t=0)=if$ by virtue of the sum rule $A(\mathbf{k},t=0;T)=1$. Also, if there were no scattering so that $A\equiv A_U$, (2.40) would automatically satisfy the kinetic equation (2.14), whose right-hand side would vanish.

Unfortunately, it is not clear that this is a correct procedure, because a system in a nonzero electric field will be in a very different state depending on whether there is scattering or not, unlike a system in equilibrium. Lipavsky, Spivack, and Velicky[19] have recently introduced a more systematic way to construct an *ansatz*. This can be written symbolically as

$$G^<(1,2)=\int d3[F(1,3)G^a(3,2)-G^r(1,3)F(3,2)] , \quad (2.41)$$

where

$$F(1,2)\equiv F(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) =\rho(\mathbf{r}_1,\mathbf{r}_2;t_1)\delta(t_1-t_2) . \quad (2.42)$$

For a uniform, constant field and using the transformation [(2.25) and (2.26)] to gauge-invariant functions, this *ansatz* reduces to

$$G^<(\mathbf{k},t)=iA(\mathbf{k},t)f(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}|t|) . \quad (2.43)$$

This can also be written in terms of reduced functions by factoring $A_U(\mathbf{k},t)$ from both sides:

$$g^<(\mathbf{k},t)=ia(\mathbf{k},t)f(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}|t|) . \quad (2.44)$$

For vanishingly small electric fields this reduces to the result of Kadanoff and Baym.[17] The limits of validity of this new *ansatz* are not obvious, but its use clears up one outstanding puzzle. This puzzle was that the kinetic equation derived from the Liouville equation for the density matrix differed slightly[23] from that derived from the Kadanoff-Baym equations with the *ansatz* (2.40). The two methods agree if the *ansatz* (2.41) is used instead,[19] and we shall therefore follow this course. Ideally, one ought to verify the accuracy of an *ansatz* by applying it to all the $G^{<,>}$ functions in the kinetic equation, not just for $t=0$, and checking that A cancels from both sides. To the best of our knowledge this has never been done for a high-field problem. The properties of the final transport equation are very sensitive to the choice of *ansatz*, so this is an important point.

Note that this approximation is never needed in linear-response theory. This is clear because the fluctuation-dissipation theorem permits response functions to be calculated from properties of the ground state, where (2.12) is exact. It has also been shown to be unnecessary in the Kadanoff-Baym formalism, again to linear response only and for slowly varying applied fields.[28,30]

We have now introduced all the preliminary results

needed to solve the equation of motion for g^r (2.29), which we shall describe in the next section. After that, we go on to derive a kinetic equation valid in high electric fields, and deduce conditions under which it reduces to the Boltzmann equation.

III. RETARDED GREEN FUNCTION

In this section we shall derive a solution to Eq. (2.29), the equation of motion for $g^r(\mathbf{k},t)$. In the course of this we shall also introduce and define some important time scales in the problem, namely the collision duration time t_c and the scattering time (mean free time) τ_{sc}.

We first go through the derivation of the "$\omega=0$" approximate solution. This solution involves modified scattering rates, which we analyze next; unlike the function γ discussed in Sec. II D, these rates are not independent of the electric field. Finally, we check the limits of validity of the approximate solution.

A. Equation of motion

If there were no electric field, the right-hand side of Eq. (2.29) would be a convolution, and an exact solution could readily by found by making a Fourier transform to ω space. For nonvanishing fields $\mathbf{F}$ the right-hand side does not take the form of a convolution, and an exact solution is no longer possible. We shall derive here an approximate solution to the equation of motion, valid when the scattering is weak and for all but very small times.

It is convenient to use the spectral function $a(\mathbf{k},t)$ rather than the retarded function $g^r(\mathbf{k},t)$, because the spectral function possesses a simpler fourer transform. The relation $g^r(\mathbf{k},t)=-i\Theta(t)a(\mathbf{k},t)$ can be used to recover the retarded Green function. Equation (2.29) for $t>0$ becomes

$$\frac{\partial}{\partial t}a(\mathbf{k},t)=-\tfrac{1}{2}i\int_{t_-}^{t}d\tau[a(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau,t-\tau)\sigma^r(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}(t-\tau),\tau)+a(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,t-\tau)\sigma^r(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}(t-\tau),\tau)]\ . \tag{3.1}$$

The lower limit t_- is arbitrary, except that it must be negative, because σ^r provides a lower cutoff on τ. We now introduce additional functions

$$a_\pm(\mathbf{k},t)=a(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,t)\ , \tag{3.2a}$$

$$\sigma^r_\pm(\mathbf{k},t)=\sigma^r(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,t)\ . \tag{3.2b}$$

The right-hand side of (3.1) can be written in terms of these new functions as $-\frac{1}{2}i[I_+(\mathbf{k},t)+I_-(\mathbf{k},t)]$, where

$$I_\pm(\mathbf{k},t)=\int_{t_-}^{t}d\tau\,a_\mp(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,t-\tau)\times\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\tau)\ , \tag{3.3}$$

note the placement of $(\pm)$ and $(\mp)$. This resembles a convolution over τ, so we insert the fourier transforms of $a_\pm$ and $\sigma^r_\pm$ and carry out the integration over τ, which yields

$$\int\int\frac{d\omega_1 d\omega_2}{(2\pi)^2}e^{-i\omega_1 t}\frac{e^{i(\omega_1-\omega_2)t}-e^{i(\omega_1-\omega_2)t_-}}{i(\omega_1-\omega_2)}\times a_\mp(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,\omega_1)\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\omega_2)\ . \tag{3.4}$$

This can be simplified by replacing ω_2 by $\omega=\omega_2-\omega_1$. We now need a value for t_-. It can be shown that t_- may be an arbitrary negative quantity by using the property that $\sigma^r_\pm(\mathbf{k},\omega)$ is analytic in ω in the upper half-plane because it is a retarded function. A particularly convenient choice is to set $t_-=-t$, which reduces the exponential factor in ω to $2\sin(\omega t)/\omega$:

$$\int\frac{d\omega_1}{2\pi}e^{-i\omega_1 t}a_\mp(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,\omega_1)\times\int\frac{d\omega}{2\pi}2\frac{\sin(\omega t)}{\omega}\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\omega_1+\omega)\ . \tag{3.5}$$

Consider the integral over ω. The $\sin(x)/x$ function tends to cut off the integral for $|\omega|>\pi/t$. If $\sigma^r_\pm(\mathbf{k},\omega)$ is slowly varying as a function of ω over this interval, it can be taken out of the integral with ω set to zero. We shall assume for now that this can be done, and return to check the validity in the next section. The remaining integral over ω yields unity, so (3.5) becomes approximately

$$\int\frac{d\omega_1}{2\pi}e^{-i\omega_1 t}a_\mp(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,\omega_1)\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\omega_1)\ . \tag{3.6}$$

Again we shall assume, and justify later, that $\sigma^r_\pm$ is a much less rapidly varying function of ω than $a_\pm$, so that it may be taken out of the integral and evaluated at $\omega=\omega_\mp(\mathbf{k}\pm\frac{1}{2}e\mathbf{F}t)$, the frequency at which $a_\mp(\mathbf{k}\pm\frac{1}{2}e\mathbf{F}t,\omega)$ is peaked. We shall also assume, and show later, that $\omega_\pm(\mathbf{k})$ may be set to zero. The remaining integral simply inverts the fourier transform of $a_\pm$, so

$$I_\pm(\mathbf{k},t)=\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\omega=0)a_\mp(\mathbf{k}\pm e\mathbf{F}t,t)=\sigma^r_\pm(\mathbf{k}\mp\tfrac{1}{2}e\mathbf{F}t,\omega=0)a(\mathbf{k},t)\ . \tag{3.7}$$

With this form for $I_\pm$, the integration of (3.1) is trivial. The result is

$$a(\mathbf{k},t)=\exp\left[-\tfrac{1}{2}i\int_0^t d\tau[\sigma^r_+(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,\omega=0)+\sigma^r_-(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau,\omega=0)]\right]\ , \tag{3.8}$$

which obeys the boundary condition $a(\mathbf{k},t=0)=1$.

A problem now arises in defining scattering rates $\gamma_\pm(\mathbf{k},\omega)$. There are two possible ways in which this might be done

$$\gamma_\pm(\mathbf{k},\omega)=-2\,\mathrm{Im}\sigma^r_\pm(\mathbf{k},\omega) \tag{3.9a}$$

or

$$\sigma^r_\pm(\mathbf{k},t)=-i\Theta(t)\gamma_\pm(\mathbf{k},t)\ . \tag{3.9b}$$

Usually these two are equivalent but this is not true for

the "±" functions, because $\sigma^a_+(\mathbf{k},-t)=[\sigma^r_-(\mathbf{k},t)]^*$, not $[\sigma^r_+(\mathbf{k},t)]^*$. This means that $\gamma_\pm(\mathbf{k},\omega)$ will not be purely real if (3.9b) is used to define $\gamma_\pm(\mathbf{k},t)$. As $\gamma_\pm(\mathbf{k},\omega)$ plays the more important part in our analysis, we shall adopt the definition (3.9a). The real part of $\sigma^r_\pm(\mathbf{k},\omega)$, giving the renormalization of the single-particle energies, is not expected to have any significant effects in the systems under consideration. We shall therefore drop it, and replace $\sigma^r_\pm$ by $-\frac{1}{2}i\gamma_\pm$ everywhere. Most of the phase variation of A is in A_U; it is only the small correction to this caused by the electron-phonon scattering that we are neglecting. The approximate solution (3.8) for a becomes

$$a(\mathbf{k},t)=\exp\left[-\tfrac{1}{4}\int_0^t d\tau[\gamma_+(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}t,\omega=0)+\gamma_-(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}t,\omega=0)]\right] \quad (3.10)$$

for $t>0$. This can be continued to negative times using $a(\mathbf{k},-t)=a^*(\mathbf{k},t)$, which means that this approximation to $a(\mathbf{k},t)$ is real and symmetric in time.

We shall now investigate how the modified scattering rates $\gamma_\pm$ differ from γ, and go back to check the conditions under which this approximate solution is valid.

B. Scattering rates with broadening

It was shown in Sec. II D that the reduced scattering rate $\gamma(\mathbf{k},\omega)$ is independent of the electric field in the special case of parabolic bands and a constant field. Unfortunately the solution to the equation of motion for g^r derived above involves modified self-energies $\sigma^r_\pm(\mathbf{k},\omega)$. These, as we shall see, are not independent of the electric field, although it is interesting to note that the broadening of the spectral function is not responsible for this.

The modified self-energies were defined by

$$\sigma^r_\pm(\mathbf{k},\omega)=\int dt\, e^{i\omega t}\sigma^r_\pm(\mathbf{k},t)=\int dt\, e^{i\omega t}\sigma^r(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,t) \quad (3.11)$$

and the equivalent of Eq. (2.35) is

$$\sigma^r_\pm(\mathbf{k},\omega)=\pi\sum_{\mathbf{q},\eta}|M_\mathbf{q}|^2[N_\mathbf{q}+\tfrac{1}{2}(1+\eta)]\frac{-i}{\pi}\int_0^\infty dt\exp\left[i\left[\omega t-\eta\Omega_\mathbf{q}t+\int_0^t d\tau[\varepsilon(\mathbf{k}\pm e\mathbf{F}\tau)-\varepsilon(\mathbf{k}+\mathbf{q}\pm e\mathbf{F}\tau)]\right]\right]. \quad (3.12)$$

The main change from (2.35) is in the limits on the integral over τ in the exponent: this apparently trivial difference has a profound effect, because $\mathbf{F}$ no longer drops out after integration. For parabolic bands the result is

$$\frac{1}{|\alpha|^{1/2}}\left[-ig\left[\pm\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]\pm\mathrm{sgn}(\alpha)f\left[\pm\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]\right], \quad (3.13)$$

where

$$\alpha=\pi\hbar^2\frac{1}{m}e\mathbf{F}\cdot\mathbf{q} \quad (3.14)$$

gives the "broadening" due to the electric field, and

$$\Delta=\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})+\eta\Omega_\mathbf{q}-\omega\ . \quad (3.15)$$

The functions $f(z)$ and $g(z)$ are associated with Fresnel integrals (Ref. 29, p. 300).

It was pointed out in Sec. III A that the definition of a scattering rate is slightly ambiguous when the (±) functions are used, and we chose to define $\gamma_\pm(\mathbf{k},\omega)=-2\,\mathrm{Im}\sigma^r_\pm(\mathbf{k},\omega)$. The scattering rates are therefore

$$\gamma_\pm(\mathbf{k},\omega)=2\pi\sum_{\mathbf{q},\eta}|M_\mathbf{q}|^2(N_\mathbf{q}+\tfrac{1}{2}[1+\eta])\times\frac{1}{|\alpha|^{1/2}}g\left[\pm\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]. \quad (3.16)$$

These scattering rates differ from $\gamma(\mathbf{k},\omega)$ in having the broadened g function replacing the δ function for energy conservation. The width of this function can be taken as $|\alpha|^{1/2}$, proportional to $F^{1/2}$. Thus the electric field is modifying the scattering rates through the intracollisional field effect.

To assess the importance of this broadening, we ignore the fact that α depends on $\mathbf{q}$, and rewrite (3.16) to express $\gamma_\pm$ in terms of γ [Eq. (2.36)] as

$$\gamma_\pm(\mathbf{k},\omega)=\int d\omega'\gamma(\mathbf{k},\omega+\omega')\times\frac{1}{|\alpha|^{1/2}}g\left[\pm\mathrm{sgn}(\alpha)\frac{\omega'}{|\alpha|^{1/2}}\right]. \quad (3.17)$$

This form shows that the broadening causes $\gamma(\mathbf{k},\omega)$ to be averaged over a range $|\alpha|^{1/2}$ of energies to give the modified rates $\gamma_\pm(\mathbf{k},\omega)$. We now define the important time scale t_c, the collision duration time, through the energy scale on which $\gamma(\mathbf{k},\omega)$ varies near $\omega=0$:

$$t_c^{-1}\left|\frac{\partial}{\partial\omega}\gamma(\mathbf{k},\omega)\right|_{\omega=0}=\gamma(\mathbf{k},\omega=0) \quad (3.18)$$

or

$$t_c=\left|\frac{\partial}{\partial\omega}\ln\gamma(\mathbf{k},\omega)\right|_{\omega=0}. \quad (3.19)$$

This collision-duration time is loosely related to that defined in scattering theory, as we show in Appendix B. The name is perhaps somewhat misleading: One should be careful about interpreting t_c as the time during which

the electron and phonon interact.

The convolution of γ with g in Eq. (3.17) will have a negligible effect provided that $|\alpha|^{1/2} \ll t_c^{-1}$. It is found in Appendix A that a typical value of t_c is 10^{-15} s, so $t_c^{-1} \approx 1$ eV. The broadening induced by the electric field does not approach this until $F \approx 1$ GV m^{-1}. The broadening is therefore almost always unimportant in conventional semiconductors, which means that the simpler function γ may be used instead of $\gamma_\pm$.

A similar argument can be made for the accuracy of calculating the self-energies with an expression that is not self-consistent, as discussed before Eq. (2.35). In a self-consistent evaluation, the full Green function, rather than one that does not include scattering, would be used within the self-energy. The integrand in Eq. (3.12) would then contain an additional decay term, roughly of the form $e^{-t/\tau_{sc}}$. This would tend to broaden the function for energy conservation, in the same way as the electric field, giving it a width of τ_{sc}^{-1}. Provided that $\tau_{sc} \gg t_c$, this broadening can be neglected, and it is accurate to calculate the self-energies using Green functions that do not themselves contain scattering.

The above arguments show that $\gamma_\pm$ may be replaced by γ with negligible loss of accuracy in a material with parabolic bands. As a final simplification [see Eq. (2.36)], $\gamma(\mathbf{k},\omega=0)$ is identical to $\Gamma(\mathbf{k})$, the total semiclassical scattering-out rate for an electron with wave vector $\mathbf{k}$ [Eq. (1.2)]. With this substitution, we obtain the final form of the "$\omega=0$" solution for $g^r(\mathbf{k},t)$:

$$g^r(\mathbf{k},t) = -i\Theta(t)a(\mathbf{k},t) ,$$
$$a(\mathbf{k},t) = \exp\left[-\tfrac{1}{2}\int_{-|t|/2}^{|t|/2} d\tau\, \Gamma(\mathbf{k}+e\mathbf{F}\tau)\right] . \tag{3.20}$$

We shall now go back to check the validity of the approximations used in deriving this solution.

C. Validity of the approximate solution

At two points in the above derivation it was necessary to assume that $\sigma_\pm(\mathbf{k},\omega)$ was a "slowly varying" function of ω. This will now be made more quantitative. The analysis relies heavily on the collision-duration time defined above [Eqs. (3.18) and (3.19)] in such a way that t_c^{-1} is the scale on which $\gamma(\mathbf{k},\omega)$ varies as a function of ω.

First, following the results of Sec. III B, we replace $\sigma_\pm^r$ by $-\frac{1}{2}i\gamma$ everywhere. In Eq. (3.5), γ was required (having replaced $\sigma_\pm^r$) over a range of energy of order π/t. It will be valid to treat γ as constant, and take it out of the integral, provided that this range of energy is much smaller than that on which $\gamma(\mathbf{k},\omega)$ varies, t_c^{-1}, i.e., provided that $t \gg t_c$. The approximate solution is therefore invalid for very small times (insignificantly small, in practice).

In simplifying Eq. (3.6), it was assumed that $a_\pm$ is a more rapidly varying function of ω than γ. The scattering time, or mean free time, τ_{sc} is defined as the time scale on which $|a(\mathbf{k},t)|^2$ decays to $1/e$ of its value at zero time:

$$|a(\mathbf{k},\tau_{sc})|^2 = 1/e . \tag{3.21}$$

The Fourier transforms $a_\pm(\mathbf{k},\omega)$ will therefore have a characteristic energy scale τ_{sc}^{-1}, and it follows that it will be valid to treat γ as slowly varying provided that $\tau_{sc}^{-1} \ll t_c^{-1}$, or $t_c \ll \tau_{sc}$. The numerical calculations in Appendix A show that this inequality is well fulfilled (by some 3 orders of magnitude) in typical semiconductors over a wide range of fields.

Finally, we must justify setting $\omega_\pm(\mathbf{k})$, the frequency at which $a_\pm(\mathbf{k},\omega)$ is peaked, to zero. It was pointed out above that the approximate solution for $a(\mathbf{k},t)$ is symmetric in time, which implies that $a(\mathbf{k},\omega)$ is also real and symmetric in ω. Provided that $a(\mathbf{k},\omega)$ has only a single peak [like a Lorentzian shape in the simplest case, where $\Gamma(\mathbf{k})$ is constant], this peak must be at $\omega=0$. Now,

$$a_\pm(\mathbf{k},\omega) = \int dt\, e^{i\omega t} a_\pm(\mathbf{k},t)$$
$$= \int dt\, e^{i\omega t} a(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}t,t) . \tag{3.22}$$

Expand the $\mathbf{k}$ argument of $a(\mathbf{k}\pm\frac{1}{2}e\mathbf{F}t,t)$ to get

$$a_\pm(\mathbf{k},\omega) = \int dt\, e^{i\omega t}[a(\mathbf{k},t) \pm \tfrac{1}{2}e\mathbf{F}\cdot\nabla_k a(\mathbf{k},t)t + \cdots] \tag{3.23}$$

$$= a(\mathbf{k},\omega) \mp \tfrac{1}{2}ie\mathbf{F}\cdot\nabla_k \frac{\partial}{\partial\omega} a(\mathbf{k},\omega) + \cdots . \tag{3.24}$$

The frequency $\omega_\pm(\mathbf{k})$ at which $a_\pm(\mathbf{k},\omega)$ is peaked will be shifted away from zero by the corrections to $a(\mathbf{k},\omega)$ in (3.24). The energy scale with which $\omega_\pm(\mathbf{k})$ should be compared is t_c^{-1}, the scale on which $\gamma(\mathbf{k},\omega)$ is sensitive to changes in ω, since this argument is where $\omega_\pm(\mathbf{k})$ appears. Equation (3.24) involves the electric field directly, and setting $\omega_\pm(\mathbf{k})$ to zero can therefore be valid in "low" fields only. To estimate the maximum field in which this is valid, we take the very rough approximation

$$a(\mathbf{k},\omega) \approx \frac{\Gamma(\mathbf{k})}{\omega^2 + \frac{1}{4}\Gamma^2(\mathbf{k})} . \tag{3.25}$$

Solving Eq. (3.24) for the peak in $a_\pm(\mathbf{k},\omega)$ and using the scattering rates from Appendix A, we find

$$\omega_\pm(\mathbf{k})/t_c^{-1} \approx 3\frac{e}{m}Fkt_c^2 . \tag{3.26}$$

Setting $k = 0.1a_0^{-1}$, this ratio is negligible for fields of less than about 1 GV m^{-1}, so it is accurate to set $\omega_\pm(\mathbf{k})$ to zero over a wide range of electric fields.

In summary, the "$\omega=0$" solution for $g^r(\mathbf{k},t)$ [Eq. (3.20)] is valid for times much greater than the collision-duration time t_c. It is limited to weak scattering, in the sense that the collision-duration time must be much smaller than the mean time between collisions τ_{sc} (this is analogous to the assumption in Boltzmann theory that collisions should be instantaneous). It is interesting to note that the latter condition is the same as that claimed by Lipavsky *et al.*[19] for the validity of the *ansatz* (2.41).

Substituting the "$\omega=0$" solution, the definition of τ_{sc} [Eq. (3.21)] becomes

$$\int_{-\tau_{sc}/2}^{\tau_{sc}/2} d\tau\, \Gamma(\mathbf{k}+e\mathbf{F}\tau) = 1 . \tag{3.27}$$

This equation is solved numerically for τ_{sc} in Appendix A. Significant values of τ are around $\frac{1}{2}\tau_{sc}$, so t_c in Ap-

pendix A is defined in terms of $\gamma(\mathbf{k}+\frac{1}{2}e\mathbf{F}\tau_{sc},\omega)$.

Our definition of t_c is in terms of the scattering rate $\gamma(\mathbf{k},\omega)$. This contains contributions from the density of states as well as from matrix elements, and is therefore more general than the definition often used.[31]

The simplification that $\gamma_\pm$ may be replaced by the semiclassical rates, which are independent of the electric field, relies on $\varepsilon(\mathbf{k})$ being parabolic. If a tight-binding (bounded) band is considered instead, $\gamma_\pm(\mathbf{k},\omega)$ shows structure reflecting transitions between levels of a Stark ladder, and may be very different from $\Gamma(\mathbf{k})$.

Having obtained a solution of the "single-particle" part of the problem, we now study the equation for $G^<$ which contains information on the "distribution" properties of the system.

IV. INTEGRAL TRANSPORT EQUATION

In this section we shall derive the final transport equation in integral form. Only electric fields that are constant in space and time will be considered. The last section dealt with finding a solution to the equation of motion for $g^r(\mathbf{k},t)$. We shall now use this solution to reduce the equation of motion for $g^<(\mathbf{k},t)$ to a transport equation for $f(\mathbf{k})$, and go on to determine the conditions under which this reduces to the Boltzmann equation.

The kinetic equation (2.27) for $g^<(\mathbf{k},t=0)$ becomes

$$\begin{aligned} f(\mathbf{k})=\sum_{\mathbf{q},\eta} |M_\mathbf{q}|^2(N_\mathbf{q}+\tfrac{1}{2}[1+\eta])\int_0^\infty dt_1\int_0^\infty dt_2 f[\mathbf{k}-\mathbf{q}-\tfrac{1}{2}e\mathbf{F}(t_1+t_2)-\tfrac{1}{2}e\mathbf{F}\,|\,t_1-t_2\,|\,] \\ \times a(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}t_1,t_1)a(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}t_2,-t_2) \\ \times a[\mathbf{k}-\mathbf{q}-\tfrac{1}{2}e\mathbf{F}(t_1+t_2),t_2-t_1] \\ \times e^{i\eta\Omega_\mathbf{q}(t_2-t_1)}A_U^{-1}[\mathbf{k}-\tfrac{1}{2}e\mathbf{F}(t_1+t_2),t_2-t_1] \\ \times A_U[\mathbf{k}-\mathbf{q}-\tfrac{1}{2}e\mathbf{F}(t_1+t_2),t_2-t_1]\,, \end{aligned} \tag{4.1}$$

where we have used (2.34a) for the self-energy $\sigma^<(\mathbf{k},t)$ and have made the *ansatz* (2.44) to replace $g^<(\mathbf{k},t)$ within the self-energy. Substituting the solution (3.20) obtained in the preceding section for the spectral function gives

$$\begin{aligned} f(\mathbf{k})=\sum_{\mathbf{q},\eta}|M_\mathbf{q}|^2[N_\mathbf{q}+\tfrac{1}{2}(1+\eta)] \\ \times\int_0^\infty dt_1\int_0^\infty dt_2 f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t_{\max}) \\ \times\exp\left[-\tfrac{1}{2}\left[\int_0^{t_1}d\tau\,\Gamma(\mathbf{k}-e\mathbf{F}\tau)+\int_0^{t_2}d\tau\,\Gamma(\mathbf{k}-e\mathbf{F}\tau)\right.\right. \\ \left.\left.+\int_{t_{\min}}^{t_{\max}}d\tau\,\Gamma(\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau)\right]\right] \\ \times\exp\left[-i\int_{t_2}^{t_1}d\tau[\varepsilon(\mathbf{k}-e\mathbf{F}\tau)-\varepsilon(\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau)+\eta\Omega_\mathbf{q}]\right]\,, \end{aligned} \tag{4.2}$$

where $t_{\max}$ and $t_{\min}$ are the larger and smaller of t_1 and t_2; interchanging t_1 and t_2 turns the integrand into its complex conjugate. Define $t=t_{\max}$ and $\tau=t-t_{\min}$, after which $f(\mathbf{k})$ becomes

$$2\pi\sum_{\mathbf{q},\eta}|M_\mathbf{q}|^2[N_\mathbf{q}+\tfrac{1}{2}(1+\eta)]\int_0^\infty dt\,f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)\exp\left[-\int_0^t d\tau'\Gamma(\mathbf{k}-e\mathbf{F}\tau')\right]S(\Delta)\,, \tag{4.3}$$

where

$$\begin{aligned} S(\Delta)=\frac{1}{\pi}\int_0^t d\tau\cos\left[\int_0^\tau d\tau'[\varepsilon(\mathbf{K}+e\mathbf{F}\tau')-\varepsilon(\mathbf{K}-\mathbf{q}+e\mathbf{F}\tau')+\eta\Omega_\mathbf{q}]\right] \\ \times\exp\left[-\tfrac{1}{2}\int_0^\tau d\tau'[\Gamma(\mathbf{K}-\mathbf{q}+e\mathbf{F}\tau')-\Gamma(\mathbf{K}+e\mathbf{F}\tau')]\right]\,, \end{aligned} \tag{4.4}$$

and

$$\Delta=\varepsilon(\mathbf{K})-\varepsilon(\mathbf{K}-\mathbf{q})+\eta\Omega_\mathbf{q} \tag{4.5}$$

with $\mathbf{K}=\mathbf{k}-e\mathbf{F}t$. The significance of $S(\Delta)$ is that it replaces the δ function $\delta(\Delta)$ of the golden rule; we have suppressed the dependence of S and Δ on other parameters to maintain clarity. For parabolic bands, $S(\Delta)$ becomes

$$\frac{1}{\pi}\int_0^t d\tau\cos\left[\Delta\tau+\frac{1}{2\pi}\alpha\tau^2\right]\exp\left[-\tfrac{1}{2}\int_0^\tau d\tau'[\Gamma(\mathbf{K}-\mathbf{q}+e\mathbf{F}\tau')-\Gamma(\mathbf{K}+e\mathbf{F}\tau')]\right]\,, \tag{4.6}$$

where α is the broadening induced by the electric field introduced previously [Eq. (3.14)]:

$$\alpha=\pi\hbar^2\frac{e}{m}\mathbf{F}\cdot\mathbf{q}\ . \tag{4.7}$$

We shall now examine the behavior of $S(\Delta)$ in more detail.

Equation (4.6) contains a decaying term, exponential with argument in large parentheses, within the integral over τ. The detailed form of this decay is not correct, because the equation of motion for g^r was not solved self-consistently; one might have expected to see the sum, rather than the difference, of the two Γ's. Although we do not expect this decay to be important, as we showed for g^r in Sec. III B, we shall estimate its effect by replacing equation (4.6) by a "worst-case" approximation:

$$S(\Delta)\approx\frac{1}{\pi}\int_0^t d\tau\, e^{-\tau/\tau_{sc}}\cos\left[\Delta\tau+\frac{1}{2\pi}\alpha\tau^2\right]\ . \tag{4.8}$$

The important values of the time t are set by the exponential decay in (4.3), and are of order τ_{sc}. $S(\Delta)$ behaves qualitatively differently depending on the relative magnitudes of τ_{sc}^{-1} and $|\alpha|^{1/2}$. If $|\alpha|^{1/2}\ll\tau_{sc}^{-1}$, the limit of small electric fields, we can drop α from the integral to obtain

$$S(\Delta)\approx\frac{\tau_{sc}^{-1}}{\pi}\frac{1}{\Delta^2+\tau_{sc}^{-2}}\ , \tag{4.9}$$

a Lorentzian of width τ_{sc}^{-1} (we have set the upper limit t of the integral to infinity). In the opposite limit of large electric fields we can drop the decay in (4.8) and get

$$S(\Delta)\approx\frac{1}{|\alpha|^{1/2}}g\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]\ , \tag{4.10}$$

where $g(x)$ is an auxilliary function associated with Fresnel integrals (Ref. 29, p. 300). The approximation of replacing the upper limit by infinity is good in this limit because the significant contributions to the integral over τ come from times less than $|\alpha|^{-1/2}$, which is less than τ_{sc}, the most significant time in the integral over t. The width of (4.10) can be taken as $|\alpha|^{1/2}$. To get an estimate of when the two limits (4.9) and (4.10) cross, we use a typical value $\tau_{sc}\approx10^{-12}$ s (see Appendix A) and set q within α to be a thermal wave vector. The crossover is found to be at $F\approx30$ kV m^{-1} for a conventional semiconductor at room temperature, so the electric field provides the dominant broadening in S even for modest strengths.

Now, $S(\Delta)$ replaces the semiclassical δ function for energy conservation in the sum over scattering rates and $f(\mathbf{k})$. The scattering rates are sensitive to blurring of the energy-conserving δ function only on an energy scale of t_c^{-1} which is very large (≈1 eV), as we saw in Sec. III B. The distribution function $f(\mathbf{k})$, on the other hand, varies on an energy scale k_BT (this should contain some "effective temperature" of the electrons rather than that of the lattice). This means that $S(\Delta)$ can be replaced by $\delta(\Delta)$, to regain the Boltzmann equation, only if the width of $S(\Delta)$ is much less than k_BT. These inequalities are considered in more detail in Appendix C. Thus we have the following condition for the validity of the Boltzmann equation:

$$k_BT\gg\begin{cases}1/\tau_{sc} & \text{if } 1/\tau_{sc}>|\alpha|^{1/2}\ ,\\ |\alpha|^{1/2} & \text{if } 1/\tau_{sc}<|\alpha|^{1/2}\ .\end{cases} \tag{4.11}$$

In summary, the condition for the validity of the Boltzmann equation in small electric fields is $1/\tau_{sc}\ll k_BT$. Taking a typical value of τ_{sc} to be 10^{-12} s, this condition is easily satisfied at room temperature. When the electric field is large, so that $|\alpha|^{1/2}>\tau_{sc}^{-1}$, the condition for the validity of the Boltzmann equation, $|\alpha|^{1/2}\ll k_BT$, is more restrictive. This condition can be violated at moderate electric fields of around 3 MV m^{-1} at room temperature, taking the effective mass to be 0.2. Note that the effective temperature of the electrons will rise in a strong electric field, so this estimate of when the Boltzmann equation fails is likely to give too small an electric field. These results agree with those of Barker and Ferry.[13]

For higher electric fields, one must use the broadening scattering-in rates, and the transport equation becomes

$$f(\mathbf{k})=2\pi\sum_{\mathbf{q},\eta}|M_{\mathbf{q}}|^2[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\int_0^\infty dt\exp\left[-\int_0^t d\tau'\Gamma(\mathbf{k}-e\mathbf{F}\tau')\right]f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)$$
$$\times\frac{1}{|\alpha|^{1/2}}g\left[\mathrm{sgn}(\alpha)\frac{\varepsilon(\mathbf{k}-e\mathbf{F}t)-\varepsilon(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)+\eta\Omega_{\mathbf{q}}}{|\alpha|^{1/2}}\right]\ , \tag{4.12}$$

an integral equation with the same form of exponential scattering-out term as in the Boltzmann equation. This means that it should be possible to solve it using similar numerical techniques.

A final comment concerns the *ansatz*. Our results are very sensitive to the choice made for this. If the more straightforward *ansatz*, Eq. (2.40), were used instead of (2.43), no intracollisional effect would be found, and the scattering rates appearing in the kinetic equation would not be broadened by the electric field. We have more to say about this in Appendix C; it explains why our conclusions differ so strongly from those of Khan and Wilkins,[16] who also used the integral transport equations.

V. CONCLUSIONS

We have studied quantum-mechanical transport equations for high electric fields, derived a new integral trans-

port equation, and determined under what conditions this reduces to the semiclassical Boltzmann equation. Two important time scales arose in this problem: the mean free time τ_{sc} and the collision duration time t_c, and two energy scales: one associated with the electric field, $|\alpha|^{1/2}$, and one characterizing the width of the distribution function, k_BT. All our results require that t_c be the smallest time scale in the problem: $t_c \ll \tau_{sc}, |\alpha|^{-1/2}, (k_BT)^{-1}$. Both the approximate solution of the equation of motion for the retarded Green function and the *ansatz* for $G^<(\mathbf{k},t)$ fail if this inequality is violated, but it is usually satisfied very easily in conventional semiconductors. The Boltzmann equation is valid provided that k_BT is the largest of the remaining energy scales: $k_BT \gg \tau_{sc}^{-1}, |\alpha|^{1/2}$. The condition for low electric fields, $k_BT \gg \tau_{sc}^{-1}$, is also required for the quasiparticle *ansatz* (Sec. II E) to hold. The Boltzmann equation fails in high electric fields when the condition $k_BT \gg |\alpha|^{1/2}$ is violated, the critical field being a few MV m^{-1} in a typical semiconductor. In higher fields, the Boltzmann equation can be replaced by a transport equation where the scattering-in term contains a broadened function rather than a δ function for energy conservation. The integral form of this equation differs little from the Boltzmann equation and should be amenable to similar numerical techniques to solve it. This would provide detailed information on the influence of the intracollisional field effect on the distribution function and transport properties.

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APPENDIX A: NUMERICAL CHECK OF TIME SCALES

In this appendix we present the results of numerical computations of the collision duration time t_c [Eq. (3.19)] and of the scattering time τ_{sc} [Eq. (3.27)]. For these calculations we shall use parabolic bands, $\varepsilon(\mathbf{k})=k^2/2m$. A value 0.22 is taken for the effective mass, corresponding to the L valley in germanium, but the qualitative results are not sensitive to this choice. We have considered nonpolar optic-phonon scattering, with a dispersionless phonon frequency $\Omega_{op}=37$ meV, appropriate for germanium. The equilibrium scattering rate is given by

$$-2\,\mathrm{Im}\Sigma^r(\mathbf{k},\omega)=\frac{(D_tK)^2m^{3/2}}{2^{1/2}\pi\rho\Omega_{op}}\sum_{\eta=\pm1}[N(\Omega_{op})+\tfrac{1}{2}(1+\eta)]\sqrt{\omega-\eta\Omega_{op}}\,\Theta(\omega-\eta\Omega_{op})\ . \tag{A1}$$

See Ref. 3, Eq. (3.72), for a description of this equation and the meaning of the symbols. Values of the parameters were also taken from this reference (Table VI of Ref. 3). The reduced scattering rate γ in equilibrium is related to this self-energy by

$$\gamma(\mathbf{k},\omega)=-2\,\mathrm{Im}\Sigma^r(\mathbf{k},\varepsilon(\mathbf{k})+\omega)\ , \tag{A2}$$

whence

$$\gamma(\mathbf{k},\omega)=\Lambda\sum_{\eta=\pm1}[N(\Omega_{op})+\tfrac{1}{2}(1+\eta)]\sqrt{\omega+\varepsilon(\mathbf{k})-\eta\Omega_{op}}\times\Theta(\omega+\varepsilon(\mathbf{k})-\eta\Omega_{op})\ , \tag{A3}$$

where $\Lambda=1.8\times10^{12}$ eV$^{-1/2}$s^{-1} with our parameters.

In this appendix we show the results of calculations of $t_c(\mathbf{k}+\frac{1}{2}e\mathbf{F}\tau_{sc})$, defined by

$$\left|\frac{\partial}{\partial\omega}\ln\gamma(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau_{sc},\omega)\right|_{\omega=0}\ , \tag{A4}$$

and of the scattering time $\tau_{sc}(\mathbf{k},\mathbf{F})$ which is obtained from Eq. (3.27):

$$\int_{-\tau_{sc}/2}^{\tau_{sc}/2}d\tau\,\gamma(\mathbf{k}+e\mathbf{F}\tau,\omega=0)=1\ . \tag{A5}$$

Figure 2 shows τ_{sc} and t_c defined in this way plotted against the strength of the electric field, F. We observe that both t_c and τ_{sc} vary little with the strength of the field up to $F\approx10^8$ V m^{-1}. In this range τ_{sc} is of order 10^{-12} s while t_c is of order 10^{-15} s. The condition $t_c \ll \tau_{sc}$ is well satisfied even for high electric fields.

Figure 3 shows τ_{sc} and t_c as a function of the wave vector $\mathbf{k}$. Again we see that the condition $t_c \ll \tau_{sc}$ is easily

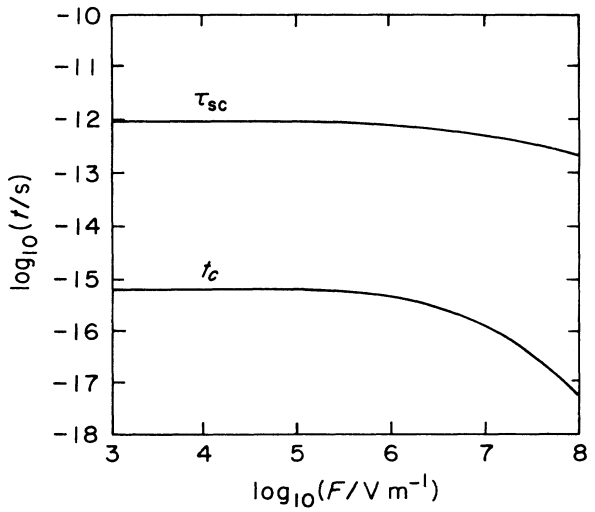

FIG. 2. Mean free time τ_{sc} and collision-duration time t_c as a function of the strength of the electric field F. The temperature is 273 K and the wave vector $k=0.1a_0^{-1}$.

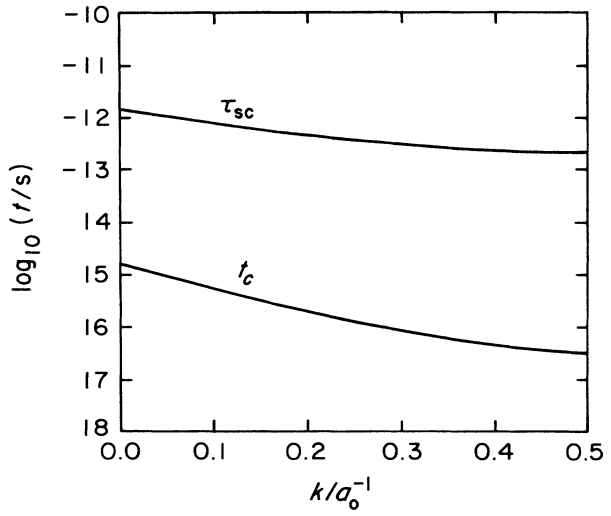

FIG. 3. Mean free time τ_{sc} and collision-duration time t_c as a function of the wave vector k, measured in inverse Bohr radii a_0^{-1}. The temperature is 273 K, $F=1$ MV m^{-1}, and **F** and **k** are parallel.

satisfied. The electric field **F** and the wave vector **k** were taken to be parallel.

Although these calculations are very simplified and use parabolic bands, the results are not expected to change qualitatively in more complicated situations or in other materials.

APPENDIX B: COLLISION-DURATION TIME

In the main body of the paper we defined an important time scale t_c which we associated with "collision duration" [Eq. (3.19)]. In this appendix we try to interpret t_c by comparing it with the "collision delay time" used in the theory of elastic scattering.

The collision delay time t_c^s can be obtained from the T matrix,

$$t_c^s=\frac{\partial}{\partial E}\arg\langle \mathbf{k}' \mid T \mid \mathbf{k}\rangle \ , \tag{B1}$$

where E is the energy $\varepsilon(\mathbf{k})$, and $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ are plane waves [see, for example, Ref. 32, Eq. (7.5.28)]. This formula holds for elastic scattering from a central potential. Physically, t_c is a measure of the "extra time" that a wave packet spends around the scattering center as compared with a free wave packet. This definition of t_c^s should be taken as a qualitative definition only, since its derivation requires certain approximations about the structure of the T matrix that may not be realistic.

To make the calculation as simple as possible, we shall assume that the scattering is elastic, and calculate t_c, for a number density N_{imp} of impurities distributed at random. The potential of each impurity is short ranged, $V_0\delta(\mathbf{r}-\mathbf{r}_i)$. We shall also assume that there is no electric field. Our definition of t_c, Eq. (3.19), is in terms of the reduced function $\gamma=-2\,\mathrm{Im}\sigma^r$, but it is more convenient to use the full self-energy Σ^r in this appendix. In equilibrium the spectral function $A_U(\mathbf{k},t)$ is $\exp[-i\varepsilon(\mathbf{k})t]$, from which it is straightforward to show that

$$\gamma(\mathbf{k},\omega)=-2\,\mathrm{Im}\Sigma^r(\mathbf{k},\varepsilon(\mathbf{k})+\omega) \ . \tag{B2}$$

Our definition of t_c therefore becomes

$$t_c=\left|\frac{\partial}{\partial E}\ln[-2\,\mathrm{Im}\Sigma^r(\mathbf{k},E)]\right|_{E=\varepsilon(\mathbf{k})} \ . \tag{B3}$$

For this model, $\mathrm{Im}\Sigma^r(\mathbf{k},E)$ is well known

$$-2\,\mathrm{Im}\Sigma^r(\mathbf{k},E)=2\pi N_{\text{imp}}\mid V_0\mid^2 N(E) \ , \tag{B4}$$

where $N(E)$ is the density of electronic states (see, for example, Ref. 33, pp. 100–108). Thus

$$t_c=\frac{1}{N(E)}\left|\frac{d}{dE}N(E)\right|_{E=\varepsilon(\mathbf{k})} \ . \tag{B5}$$

To calculate the T matrix, we place an impurity with potential $V_0\delta(\mathbf{r}-\mathbf{r}_0)$ at $\mathbf{r}_0$ and calculate the Green function $G^r(\mathbf{r},\mathbf{r}')$. This is easily found to be

$$G^r(\mathbf{r},\mathbf{r}')=G_0^r(\mathbf{r},\mathbf{r}')+G_0^r(\mathbf{r},\mathbf{r}_0)\frac{V_0}{1-V_0G_0^r(\mathbf{r}_0,\mathbf{r}_0)}\times G_0^r(\mathbf{r}_0,\mathbf{r}') \tag{B6}$$

(see, for example, Ref. 34, pp. 131–134), and $G_0^r(\mathbf{r}_0,\mathbf{r}_0)$ may be written

$$G_0^r(\mathbf{r}_0,\mathbf{r}_0)=\int dE'\frac{N(E')}{E-E'+i\eta}=I(E)-i\pi N(E) \ , \tag{B7}$$

where $I(E)$ is the principal part of the integral. The T matrix is defined in terms of G by $G=G_0+G_0TG_0$, so we see that

$$T^r(\mathbf{r},\mathbf{r}';E)=\delta(\mathbf{r}-\mathbf{r}_0)\delta(\mathbf{r}'-\mathbf{r}_0)\times\frac{V_0}{1-V_0I(E)+i\pi V_0N(E)} \ . \tag{B8}$$

Now we use scattering theory [Eq. (B1)] to define the collision delay time t_c^s and assume that the potential V_0 is weak so that we need keep only terms to the lowest order in V_0. The result is

$$t_c^s=\pi\left|V_0\frac{d}{dE}N(E)\right|_{E=\varepsilon(\mathbf{k})} \ . \tag{B9}$$

Comparing t_c and t_c^s, we see that they are related but are far from identical. Both contain the derivative of the density of states, which is the only function that depends on energy when short-ranged impurities are used. However, t_c^s contains V_0 whereas t_c has no dependence at all on the strength of the potential. This means that t_c^s goes to zero as the scattering potential is made vanishingly small, as seems physically reasonable, but t_c is unaffected.

At present, we are unable to place a more physical interpretation on t_c than that provided by its original definition.

APPENDIX C: DIFFERENTIAL TRANSPORT EQUATION

All our conclusions until now have been based on the integral form of the quantum transport equations (2.16). Earlier work that predicted an important intracollisional field effect[13,20,21,26] used differential transport equations. We show in this appendix how our conclusions follow also from the differential form (2.14), again considering only a uniform, constant electric field $\mathbf{F}$ and parabolic bands. These results are then used to repeat our derivation of an integral transport equation which contains no more integrals than the Boltzmann equation, and which could be solved numerically.

1. Validity of the Boltzmann equation

In this section, we repeat our derivation of a transport equation and a set of conditions under which the Boltzmann equation is accurate, but this time we use the differential formulation of the quantum transport theory.

Written in the terms of mechanical momentum k, the kinetic equation is

$$e\mathbf{F}\cdot\nabla_k f(\mathbf{k}) = -ie\mathbf{F}\cdot\nabla_k G^<(\mathbf{k},t=0) = \int_0^\infty d\tau[\Sigma^<(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,\tau)G^>(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,-\tau)+G^>(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,\tau)\Sigma^<(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau,-\tau)-\Sigma^>G^<-G^<\Sigma^>] . \tag{C1}$$

We shall again use the Born approximation (2.33) for the self-energies, and make the *ansatz* (2.43) derived from Lipavsky *et al.*[19] to remove the unknown t dependence of $G^{<,>}$ from the RHS:

$$G^<(\mathbf{k},t)=iA(\mathbf{k},t)f(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\,|\,t\,|\,) , \qquad G^>(\mathbf{k},t)=-iA(\mathbf{k},t)[1-f(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\,|\,t\,|\,)]\approx -iA(\mathbf{k},t) . \tag{C2}$$

The collision term becomes

$$\sum_{\mathbf{q}}\int_0^\infty d\tau[P(\mathbf{k}-e\mathbf{F}\tau,\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau;\tau)f(\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau) - P(\mathbf{k}+\mathbf{q}-e\mathbf{F}\tau,\mathbf{k}-e\mathbf{F}\tau;\tau)f(\mathbf{k}-e\mathbf{F}\tau)] , \tag{C3}$$

where

$$P(\mathbf{k}+\mathbf{q},\mathbf{k};\tau)=2\pi\,|\,M_{\mathbf{q}}\,|^2\sum_\eta[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\mathrm{Re}\frac{1}{\pi}[A(\mathbf{k}+\mathbf{q}+\tfrac{1}{2}e\mathbf{F}\tau,\tau)A(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau,-\tau)e^{-i\eta\Omega_{\mathbf{q}}\tau}] . \tag{C4}$$

If $\mathbf{F}=0$ and the free-particle spectral functions are used for A, the integral over τ in (C3) collapses to a δ function and we recover the golden rule transition rates [Eq. (2.1)].

A severe problem with interpreting this equation is that τ enters in two distinct ways. The first is through the time evolution of the momenta and the second is in the spectral functions, where it represents the fact that the collisions are not considered to occur instantaneously in the quantum transport theory. To separate the two ways in which τ appears, we integrate both sides of the transport equation (C3) to get

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt\int_0^\infty d\tau[P(\mathbf{k}-e\mathbf{F}(t+\tau),\mathbf{k}-\mathbf{q}-e\mathbf{F}(t+\tau);\tau)f(\mathbf{k}-\mathbf{q}-e\mathbf{F}(t+\tau))-Pf] \tag{C5}$$

($\mathbf{k}$ is replaced by $\mathbf{k}+\mathbf{q}$ in the second Pf term). This can be verified by operating on both sides with $e\mathbf{F}\cdot\nabla_k$. After some manipulation of t and τ, (C5) takes on the attractive form

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt[\tilde{W}(\mathbf{k}-e\mathbf{F}t,\mathbf{k}-\mathbf{q}-e\mathbf{F}t;t)f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)-\tilde{W}f] . \tag{C6}$$

For comparison, the Boltzmann equation gives

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt[W(\mathbf{k}-e\mathbf{F}t,\mathbf{k}-\mathbf{q}-e\mathbf{F}t)f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)-Wf] . \tag{C7}$$

These would be of identical form if the transition rates in (C6), given by

$$\tilde{W}(\mathbf{K}+\mathbf{q},\mathbf{K},t)=\int_0^t d\tau P(\mathbf{K}+\mathbf{q},\mathbf{K},\tau) =2\pi\,|\,M_{\mathbf{q}}\,|^2\sum_\eta[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\int_0^t d\tau\,\mathrm{Re}\frac{1}{\pi}[A(\mathbf{K}+\mathbf{q}+\tfrac{1}{2}e\mathbf{F}\tau,\tau)A(\mathbf{K}+\tfrac{1}{2}e\mathbf{F}\tau,-\tau)e^{-i\eta\Omega_{\mathbf{q}}\tau}] , \tag{C8}$$

were to be independent of t and reduce to δ functions; $\mathbf{K}=\mathbf{k}-e\mathbf{F}t$. Note that we have now separated the time evolution of the momenta in the distribution functions [argument t in (C6)] from the time evolution within collisions [argument τ in (C8)]. If the electric field is neglected, and one takes the limit of completed collisions ($t\to\infty$), the transition rate

reduces simply to a convolution of the two spectral functions. This has been used[35] in investigations of collisional broadening.

We introduce the reduced spectral function by writing $A = A_U a$ [see Eq. (2.21)], and use the approximate solution derived in Sec. III for $a(\mathbf{k},t)$. After these replacements, the integral in (C8) becomes

$$S(\Delta)=\frac{1}{\pi}\int_0^t d\tau \cos\left[\int_0^\tau d\tau'[\varepsilon(\mathbf{K}+\mathbf{q}+e\mathbf{F}\tau')-\varepsilon(\mathbf{K}+e\mathbf{F}\tau')+\eta\Omega_q]\right] \times\exp\left[-\tfrac{1}{2}\int_0^\tau d\tau'[\Gamma(\mathbf{K}+\mathbf{q}+e\mathbf{F}\tau')+\Gamma(\mathbf{K}+e\mathbf{F}\tau')]\right], \tag{C9}$$

where

$$\Delta=[\varepsilon(\mathbf{K}+\mathbf{q})-\varepsilon(\mathbf{K})+\eta\Omega_q], \tag{C10}$$

the semiclassical transition energy, and unnecessary parameters in S and Δ have been suppressed in the interests of clarity. This expression replaces the δ function in the golden rule. The energies $\varepsilon(\mathbf{k})$ should really be renormalized but this is unlikely to be important, as we argued in Sec. III A. By using the "$\omega=0$" approximation for A, rather than just A_U, we are effectively calculated the self-energies $\Sigma^{<,>}$ of Fig. 1 self-consistently. While we expect this to be numerically insignificant (as we showed in Sec. III B), including the decay in the Green functions is vital for setting limits on the validity of the Boltzmann equation when the electric field is weak.

Comparing Eqs. (4.4) and (C9), we see that they are identical except that (C9) has the sum of the two Γ's whereas (4.4) has their difference. One would normally expect to see the sum, and the error in (4.4) probably arises because the "$\omega=0$" approximation is not a self-consistent solution to the equation of motion for g^r. The differential transport equation is less sensitive to such details.

As the detailed form of the decay is not important, we replace $\Gamma(\mathbf{k})$ by an average value $1/\tau_{sc}$. For parabolic bands, (C9) becomes

$$S(\Delta)\approx\frac{1}{\pi}\int_0^t d\tau\, e^{-\tau/\tau_{sc}}\cos\left[\Delta\tau+\frac{1}{2\pi}\alpha t^2\right], \tag{C11}$$

the same as (4.8), and

$$\alpha=\pi\hbar^2\frac{e}{m}\mathbf{F}\cdot\mathbf{q} \tag{C12}$$

gives the broadening due to the electric field introduced in Sec. III B, Eq. (3.14). The semiclassical limit involves neglecting the electric field ($\alpha\to 0$) and decay ($\tau_{sc}\to\infty$) within the scattering rate, and assuming that collisions are completed ($t\to\infty$). In this case, $S(\Delta)\to\delta(\Delta)$. Dropping these conditions allows S to gain a "width" w in Δ. Equation (C11) can be evaluated in terms of complex error functions but this is not very illuminating, and instead we examine its behavior in three limits to get a feel for w. When t is small,

$$S(\Delta)\sim\frac{1}{\pi}\frac{\sin\Delta t}{\Delta}, \tag{C13a}$$

so $w\approx 1/t$. For $t\to\infty$ and $F=0$,

$$S(\Delta)\sim\frac{\tau_{sc}^{-1}}{\pi}\frac{1}{\Delta^2+\tau_{sc}^{-2}}, \tag{C13b}$$

in which case $w\approx 1/\tau_{sc}$. Finally, if $t\to\infty$ and $\tau_{sc}\to\infty$,

$$S(\Delta)\sim\frac{1}{|\alpha|^{1/2}}g\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right], \tag{C13c}$$

where $g(x)$ is an auxilliary function associated with Fresnel integrals (Ref. 29, p. 300), and $w\approx|\alpha|^{1/2}$ can be taken as the width of $S(\Delta)$. For general values of t, τ_{sc}, and α, w is given by the largest of these three limiting forms. We shall now examine the scattering-out and scattering-in terms in turn, to see the effect of the broadening of $S(\Delta)$.

a. *Scattering-out term*

To examine the effect of $S(\Delta)$ having a nonzero width, we look first at the scattering out term in the kinetic equation (C6),

$$\int_0^\infty dt\, f(\mathbf{k}-e\mathbf{F}t)\sum_q\tilde{W}(\mathbf{k}+\mathbf{q}-e\mathbf{F}t,\mathbf{k}-e\mathbf{F}t;t). \tag{C14}$$

Note that this term does not include the distribution function f within the summation over $\mathbf{q}$. If $\tilde{W}$ contained exact δ functions,

$$\sum_q\tilde{W}(\mathbf{K}+\mathbf{q},\mathbf{K};t)\to\sum_q W(\mathbf{K}+\mathbf{q},\mathbf{K})=\Gamma(\mathbf{K})=\gamma(\mathbf{K},\omega=0), \tag{C15}$$

where $W(\mathbf{K}+\mathbf{q},\mathbf{K})$ is given by (2.1), $\Gamma(\mathbf{K})$ by (1.2), and $\gamma(\mathbf{K},\omega)$ by (2.36); ω sets the amount by which the semiclassical δ function for energy conservation is violated. The nonzero width w of the energy-conservation function within $\tilde{W}$ effectively causes γ to be averaged over a range of ω (the argument is the same as that in Sec. III B). The averaging is unimportant, and this procedure reduces to the use of an exact δ function, if

$$w\left|\frac{\partial}{\partial\omega}\gamma(\mathbf{k},\omega)\right|_{\omega=0}\ll\gamma(\mathbf{k},\omega=0) \tag{C16}$$

or

$$w\ll\left[\left|\frac{\partial}{\partial\omega}\ln\gamma(\mathbf{k},\omega)\right|_{\omega=0}\right]^{-1}=t_c^{-1} \tag{C17}$$

where t_c is the collision-duration time defined in Sec. III B [Eq. (3.19)]. The use of $\Gamma(\mathbf{k})$, which contains

scattering-out rates involving δ functions, will therefore be accurate provided that $w \ll 1/t_c$. This confirms the conclusions reached in Sec. III.

Next, we need to consider which of the three limiting forms for w from equations (C13a)–(C13c) is important. For small times, $w \approx t^{-1}$, while for large times w approaches the greater of τ_{sc}^{-1} and $|\alpha|^{1/2}$. The limiting form at small times, t^{-1}, is never important. This is because it provides the greatest width only for very small times, $t < \tau_{sc}, |\alpha|^{-1/2}$, which make only a small contribution to the integral over t in (C14). The important range of this integral is from zero to several times τ_{sc}. This is because τ_{sc} is a mean lifetime between scatterings, during which time the electron travels $e\mathbf{F}\tau_{sc}$ in $\mathbf{k}$ space. It is clear that the width of the distribution function in $\mathbf{k}$ space must be several times this value, otherwise a typical electron would travel further between collisions than the width of the distribution, which is absurd. Thus the significant range of t in (C14) must extend to several times τ_{sc} and the part where $t < \tau_{sc}$ is not important. In stronger electric fields, where $|\alpha|^{-1/2} < \tau_{sc}$, w is set by t^{-1} only for $t < |\alpha|^{-1/2}$ which is an even smaller fraction of the integral. Thus the limit $w \approx t^{-1}$ can be neglected, and the strength of the electric field determines which of τ_{sc}^{-1} and $|\alpha|^{1/2}$ is the important width.

When the electric field is weak, so $|\alpha|^{1/2} < \tau_{sc}^{-1}$, the Boltzmann equation will hold provided that $\tau_{sc}^{-1} \ll t_c^{-1}$, or $t_c \ll \tau_{sc}$. This inequality also means that it is unnecessary to use a Green function that itself includes scattering when calculating the scattering rate, i.e., collisional broadening is insignificant. This is a well-known condition for the Boltzmann equation to be valid in weakly-perturbed systems, and means that the time spent *within* collisions is much less than the time spent *between* collisions.

As the electric field becomes stronger, $|\alpha|^{1/2}$ will exceed τ_{sc}^{-1}. A rough value of τ_{sc}^{-1} is 5 meV. Putting a thermal wave vector $\sqrt{mk_BT}$ as a typical value of q in α, the electric field becomes more important for $F > 30$ kV m^{-1} at room temperature, taking the effective mass to be 0.2. Thus the electric field provides the critical scale even for relatively modest field strengths. A typical collision-duration time t_c is 10^{-15} s, giving a width of about 1 eV (it is possible for t_c to become much larger in some situations, near the threshold for scattering by optic phonons for example). The width induced by the electric field approaches this only for strengths of 1 GV m^{-1}. This means that $w \ll 1/t_c$, and δ functions may be used in the scattering-out rate, over a wide range of conditions.

b. Scattering-in term

We now turn to the scattering-in term. This includes the distribution function f within the summation over $\mathbf{q}$, which changes markedly the above conclusions. This is because w must now be compared with the energy scale on which f varies, namely k_BT, as well as t_c^{-1}; note that T should be some "effective temperature" in the case of hot electrons, and may be much higher than the temperature of the lattice. Since $k_BT \ll t_c^{-1}$, the widths in energy must satisfy

$$\tau_{sc}^{-1}|\alpha|^{1/2} \ll k_BT \tag{C18}$$

if transition rates involving δ functions are to be accurate, and the Boltzmann equation is to be applicable. The inequality involving τ_{sc} is also required for the *ansatz* to be valid (Sec. II E). For large electric fields, the inequality involving α is the important one. Using the same estimate for α as before, (C18) becomes

$$eF \ll \frac{1}{\pi}[m(k_BT)^3]^{1/2} \tag{C19}$$

and for $T = 300$ K the critical field is about 3 MV m^{-1}. At this point the Boltzmann equation fails.[13]

It is worth pausing briefly to ask how strongly these conclusions depend on the specific *ansatz* (2.43) used for $G^<$. If we were instead to use the straightforward generalization[23] of Kadanoff and Baym's *ansatz*, Eq. (2.40), the final results would be drastically different. The term with α in (C11) would not appear, and we would arrive at the result that the electric field has no direct effect on the validity of the Boltzmann equation. This is why our criteria for the validity of the Boltzmann equation differ so markedly from those of Khan and Wilkins.[16] If the *ansatz* (2.43) is used, the scattering rates in G^r (calculated in Sec. III) are identical to those in $G^<$ (calculated in Sec. IV), but this symmetry is broken if (2.40) is adopted instead. This provides further support for the *ansatz* of Lipavsky *et al.*[19]

It is interesting that the semiclassical form of the scattering-*out* term remains valid for a wide range of electric fields after the complete Boltzmann equation has broken down. We can capitalize on this observation to build an integral equation for $f(\mathbf{k})$ that is not too much more complicated than the Boltzmann equation.

2. Constructing an integral transport equation

We shall now derive an integral transport equation based on the results of the preceding section. Provided that $t_c \ll \tau_{sc}, |\alpha|^{-1/2}$, which is true over a wide range of conditions, the semiclassical form of the scattering-out term is adequate.

In this case, (C3) becomes

$$e\mathbf{F}\cdot\nabla_k f(\mathbf{k}) = \sum_{\mathbf{q}} \int_0^\infty d\tau\, P(\mathbf{k}-e\mathbf{F}\tau, \mathbf{k}-\mathbf{q}-e\mathbf{F}\tau;\tau) \times f(\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau) - \Gamma(\mathbf{k})f(\mathbf{k}) , \tag{C20}$$

where $\Gamma(\mathbf{k})$ is the total semiclassical scattering-out rate [Eq. (1.2)]. This can be cast as an integral equation for $f(\mathbf{k})$ in exactly the same way as the Boltzmann equation (2.3). The result is

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt\exp\left[-\int_0^t dt'\Gamma(\mathbf{k}-e\mathbf{F}t')\right]$$
$$\times\int_0^\infty d\tau P(\mathbf{k}-e\mathbf{F}(t+\tau),\mathbf{k}-\mathbf{q}-e\mathbf{F}(t+\tau);\tau)f(\mathbf{k}-\mathbf{q}-e\mathbf{F}(t+\tau))\ . \tag{C21}$$

Reordering the integrations and manipulating the time variables in the right-hand side gives

$$\sum_{\mathbf{q}}\int_0^\infty dt\, f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)\int_0^t d\tau\exp\left[-\int_0^{t-\tau}dt'\Gamma(\mathbf{k}-e\mathbf{F}t')\right]P(\mathbf{k}-e\mathbf{F}t,\mathbf{k}-\mathbf{q}-e\mathbf{F}t;\tau)\ . \tag{C22}$$

The distribution function f has been removed from the integration over τ, a vital simplification. The semiclassical result could be regained if the τ integral involved P only, and ranged from 0 to ∞. If this is to be a good approximation to (C22), $P(\mathbf{K},\mathbf{K}-\mathbf{q};\tau)$ needs to be short-ranged in τ. Now, $P(\mathbf{K}\mathbf{K}-\mathbf{q};\tau)$ is the derivative of $\tilde{W}(\mathbf{K},\mathbf{K}-\mathbf{q};\tau)$ with respect to τ [see (C8)], so P will be significant only for times until $\tilde{W}$ has reached its asymptotic value for large times. The analysis of $\tilde{W}$ [Eq. (C13)] shows that this occurs when τ reaches the smaller of τ_{sc} and $|\alpha|^{-1/2}$. The most significant values of t in (C22) are of order τ_{sc}, as argued above, so $P(\mathbf{K},\mathbf{K}-\mathbf{q};\tau)$ can indeed be taken as short-ranged in τ. Note that this approximation gets better as the electric field gets larger and $|\alpha|^{-1/2}$ gets smaller. Therefore we can set $\tau=0$ in the upper limit of the integral over t' in the scattering-out term. The integral over τ then involves just P, turning it into $\tilde{W}$:

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt\, f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)$$
$$\times\exp\left[-\int_0^t dt'\Sigma(\mathbf{k}-e\mathbf{F}t')\right]$$
$$\times\tilde{W}(\mathbf{k}-e\mathbf{F}t,\mathbf{k}-\mathbf{q}-e\mathbf{F}t;t)\ . \tag{C23}$$

This equation includes both the effect of the electric field acting during collisions, and of collisions having a nonzero duration in time. The latter effect has been shown above to be negligible, because $\tilde{W}(\mathbf{K},\mathbf{K}-\mathbf{q},t)$ assumes its asymptotic form for the most significant parts of the integral over t. In this case it is permissible to replace $\tilde{W}$ by its limits as $t\to\infty$. The result is an approximate integral equation that differs from the Boltzmann equation only in having $\tilde{W}(\mathbf{K},\mathbf{K}-\mathbf{q};t\to\infty)$ rather than $W(\mathbf{K},\mathbf{K}-\mathbf{q})$. When the electric field is large, and for parabolic bands, this can be written

$$f(\mathbf{k})=\sum_{\mathbf{q}}\int_0^\infty dt\, f(\mathbf{k}-\mathbf{q}-e\mathbf{F}t)\exp\left[-\int_0^t dt'\Gamma(\mathbf{k}-e\mathbf{F}t')\right]$$
$$\times 2\pi|M_{\mathbf{q}}|^2\sum_{\eta}[N_{\mathbf{q}}+\tfrac{1}{2}(1+\eta)]\left[\frac{1}{|\alpha|^{1/2}}g\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]\right] \tag{C24}$$

with the broadened g function replacing the δ function of semiclassical theory [Δ is given by Eq. (C10)]. This equation is identical to (4.12), and contains no more integrals than the Boltzmann equation. It should therefore be possible to implement numerical methods to solve it, and thereby gain a quantitative understanding of the intracollisional field effect.

The symmetry between the scattering-in and scattering-out rates can be made more explicit by using the somewhat more accurate expression

$$\Gamma(\mathbf{k})=\sum_{\mathbf{q}}\tilde{W}(\mathbf{k}+\mathbf{q},\mathbf{k};t\to\infty) \tag{C25}$$

for Γ instead of that in terms of $W(\mathbf{k}+\mathbf{q},\mathbf{k})$ [Eq. (1.2)]. The two definitions should give the same result provided that $t_c\ll|\alpha|^{-1/2}$, but the new one may be more convenient because the rates $\tilde{W}$ are needed in the scattering-in term. As an aside, it is perhaps misleading to describe $\tilde{W}$ as a "rate" because it is not positive definite. Also, the oscillations in $g(x)$ make it an unpleasant function to handle numerically and the inclusion of a damping term may be necessary to control this.

Finally, we can differentiate (C24) again to obtain

$$e\mathbf{F}\cdot\nabla_k f(\mathbf{k})=\sum_{\mathbf{q}}\tilde{W}(\mathbf{k},\mathbf{k}-\mathbf{q};t\to\infty)f(\mathbf{k}-\mathbf{q})$$
$$-\Gamma(\mathbf{k})f(\mathbf{k})\ . \tag{C26}$$

This differs from the Boltzmann equation (1.1), with which we started, only in having broadened g functions instead of δ functions from the golden rule. A much shorter route to this result would have been to pull f out of the integrals over τ in Eq. (C3); this means that $P(\mathbf{K},\mathbf{K}-\mathbf{q};t)$ is assumed to be a very short-ranged function of t. It is far from obvious *a priori* that P has this property, and essentially all of the above analysis is required to show that this simple approximation is the one to make.

APPENDIX D: PHYSICAL PICTURE OF THE INTRACOLLISIONAL FIELD EFFECT

The transition rates in the Boltzmann equation are calculated in the absence of an electric field, i.e., between pairs of eigenstates like $\exp[i(\mathbf{k}\cdot\mathbf{r}-\varepsilon(\mathbf{k})t]$. These have both a well-defined energy and momentum, leading to δ functions to conserve these quantities. If the electric field is taken into account when calculating the transition rates, the electronic states are no longer so simple. Consider two states which at $t=0$ have wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, and energies $\varepsilon(\mathbf{k}_1)$ and $\varepsilon(\mathbf{k}_2)$. Absorption of a phonon with wave vector $\mathbf{q}=\mathbf{k}_1-\mathbf{k}_2$ and energy $\Omega_{\mathbf{q}}=\varepsilon(\mathbf{k}_1)-\varepsilon(\mathbf{k}_2)$ could cause a transition from state 2 to state 1 in the absence of an applied electric field. When $\mathbf{F}$ is turned on, the states evolve in $\mathbf{k}$ space so that $\mathbf{k}(t)=\mathbf{k}+e\mathbf{F}t$. Their difference in momentum remains $\mathbf{q}$ at all times, but their difference in energy, $\varepsilon(\mathbf{k}_1+e\mathbf{F}t)-\varepsilon(\mathbf{k}_2+e\mathbf{F}t)$, does not in general remain constant. For parabolic bands, this difference is $\varepsilon(\mathbf{k}_1)-\varepsilon(\mathbf{k}_2)+e\mathbf{F}\cdot\mathbf{q}t/m$, which remains constant only for those phonons with $\mathbf{q}$ perpendicular to $\mathbf{F}$. The lack of a well-defined energy different destroys the δ function for energy conservation in the semiclassical rates: this is the intracollisional field effect.

This picture suggests that a modification of the golden rule might be used to calculate modified transition rates.[15] It is necessary to choose a basis for the wave functions, which in turn requires a choice of gauge. We shall use a vector potential $\mathbf{A}(t)=-\mathbf{F}t$, as was implicitly used above. Canonical momentum $\mathbf{p}$ is conserved, and the basis functions are

$$\psi(\mathbf{r},t;\mathbf{p})=\exp\left[i\left[\mathbf{p}\cdot\mathbf{r}-\int_0^t d\tau\,\varepsilon(\mathbf{p}-e\,\mathbf{A}(\tau))\right]\right]. \quad \text{(D1)}$$

We now follow the usual argument for deriving the golden rule. At $t=0$, only the state $\mathbf{p}$ is occupied. The probability $|a(\mathbf{p}+\mathbf{q},t)|^2$ that the state $\mathbf{p}+\mathbf{q}$ is occupied after a perturbation $M_{\mathbf{q}}\exp[i(\mathbf{q}\cdot\mathbf{r}-\Omega_{\mathbf{q}}t)]$ has been applied for time t is found to be

$$\left|M_{\mathbf{q}}\int_0^t dt'\exp\left[-i\int_0^{t'}d\tau[\varepsilon(\mathbf{p}+\mathbf{q}-e\,\mathbf{A}(\tau))-\varepsilon(\mathbf{p}-e\,\mathbf{A}(\tau))-\Omega_{\mathbf{q}}]\right]\right|^2. \quad \text{(D2)}$$

Concern has been raised[15] about whether a transition rate should be derived from $|a(\mathbf{p}+\mathbf{q},t)|^2$ by differentiating with respect to t or by dividing by t. It seems to us that the two definitions must agree in the limit of large times if the concept of a transition rate is to be meaningful. Using the former definition, the transition rate derived from (D2) is

$$2\pi|M_{\mathbf{q}}|^2\frac{1}{\pi}\int_0^t dt'\cos\left[\int_{t'}^t d\tau[\varepsilon(\mathbf{p}+\mathbf{q}-e\,\mathbf{A}(\tau))-\varepsilon(\mathbf{p}-e\,\mathbf{A}(\tau))-\Omega_{\mathbf{q}}]\right]. \quad \text{(D3)}$$

This closely resembles $\tilde{W}(\mathbf{p}_1,\mathbf{p}_2;t)$ [Eqs. (C8) and (C9)]; the two would become identical if $\mathbf{p}$ were replaced by $\mathbf{k}=\mathbf{p}-e\,\mathbf{A}(t)$, and the occupation numbers for the phonons were included. For parabolic bands, (D3) can be evaluated in terms of Fresnel integrals:

$$2\pi|M_{\mathbf{q}}|^2\frac{1}{|\alpha|^{1/2}}\left[\mathrm{sgn}(\alpha)\sin\left[\Delta t-\frac{\alpha}{2\pi}t^2\right]f\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]-\cos\left[\Delta t-\frac{\alpha}{2\pi}t^2\right]g\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}\right]+g\left[\mathrm{sgn}(\alpha)\frac{\Delta}{|\alpha|^{1/2}}-\frac{|\alpha|^{1/2}}{\pi}t\right]\right], \quad \text{(D4)}$$

where

$$\Delta=\varepsilon(\mathbf{p}+\mathbf{q})-\varepsilon(\mathbf{p})-\Omega_{\mathbf{q}} \quad \text{(D5)}$$

and α was defined previously [Eq. (3.14)]. This has the now-familiar f and g functions of $\Delta/|\alpha|^{1/2}$. Unfortunately, it has no well-defined limit as $t\to\infty$, showing that a transition rate cannot be defined this way. The source of the error lies in using canonical momentum $\mathbf{p}$ rather than mechanical momentum $\mathbf{k}$. A great advantage of using Green functions is that they can be made gauge invariant, unlike wave functions.

One could instead use a scalar-potential gauge with $\phi(x)=-eFx$, a method that has been extensively pursued by Herbert and Till[14] and Ziep and Keiper.[36] Eigenfunctions with well-defined energies exist in this gauge, the Airy functions:

$$\psi(x,t;E)=\left[\frac{2m}{c}\right]^{1/4}\mathrm{Ai}\left[\frac{1}{c}(eFx-E)\right]e^{-iEt}, \qquad c=\left[\frac{(eF)^2}{2m}\right]^{1/3}. \quad \text{(D6)}$$

We are considering a one-dimensional model for simplicity, and have chosen the normalization such that

$$\int dx\,\psi^*(x,t;E_1)\psi(x,t;E_2)=\delta(E_1-E_2). \quad \text{(D7)}$$

These states have the minor disadvantage that they do not carry current individually, although current-carrying wave functions can be made from superpositions of Airy

functions. In this case, the transition rate between two states with energies E_1 and E_2 due to a perturbation $M_q \exp[i(\mathbf{q}x - \Omega_q t)]$ is given by

$$2\pi \frac{m}{2\pi e F \mathbf{q}} \delta(E_2 - E_1 + \Omega_q) , \tag{D8}$$

using the usual golden rule. Note that the matrix element is independent of E_1 and E_2, because the Fourier transform of Ai(z) has contributions of equal magnitude from all of k space. While there is now always a δ function for the conservation of energy, there is not one for momentum. It seems more difficult to relate this formulation to the Boltzmann equation, although the two methods must agree when the electric field is weak.

While the intracollisional field effect has a simple physical interpretation, it seems to be difficult to do calculations in an elementary way based on this, mainly because of the problems of maintaining gauge invariance.

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[1]W. Fawcett, in *Electrons in Crystalline Solids* (International Atomic Energy Agency, Vienna, 1973).

[2]Peter J. Price, Semicond. Semimetals, **14**, 249 (1979).

[3]Carlo Jacoboni and Lino Reggiani, Rev. Mod. Phys. **55**, 645 (1983).

[4]J. R. Barker, in *Handbook of Semiconductors,* edited by W. Paul (North-Holland, Amsterdam, 1982), pp. 617–659.

[5]A. F. J. Levi, J. R. Hayes, P. M. Platzman, and W. Weigmann, Phys. Rev. Lett. **55**, 2071 (1985); A. F. J. Levi, J. R. Hayes, and R. Bhat, Appl. Phys. Lett. **48**, 1609 (1986).

[6]M. Heiblum, M. I. Nathan, D. C. Thomas, and C. M. Knoedler, Phys. Rev. Lett. **55**, 2200 (1985).

[7]K. Tomizawa, Y. Awano, N. Hashizume, and M. Kawashima, IEE (Inst. Electr. Eng.)—IERE (Inst. Electron Radio Eng.) Proc. (India) **129**, 131 (1982).

[8]A. Ghis, E. Constant, and B. Boittiaux, J. Appl. Phys. **54**, 214 (1983).

[9]P. Hesto, Surf. Sci. **132**, 623 (1983).

[10]Harold U. Baranger and John W. Wilkins, Phys. Rev. B **30**, 7349 (1984).

[11]A. P. Long, P. H. Beton, and M. J. Kelly, Semicond. Sci. Technol. **1**, 63 (1986).

[12]E. M. Conwell, in *Handbook of Semiconductors,* Ref. 4, pp. 513–561.

[13]J. R. Barker and D. K. Ferry, Phys. Rev. Lett. **42**, 1779 (1979).

[14]D. C. Herbert and S. J. Till, J. Phys. C **15**, 5411 (1982).

[15]D. Lowe, J. Phys. C **18**, L209 (1985).

[16]Furrukh S. Khan and John W. Wilkins, Semicond. Sci. Technol. **1**, 113 (1986).

[17]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Reading, Mass., 1962).

[18]L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys.—JETP **20**, 1018 (1965)].

[19]P. Lipavsky, V. Spicka, and B. Velicky, Phys. Rev. B **34**, 6933 (1986).

[20]I. B. Levinson, Zh. Eksp. Teor. Fiz. **47**, 660 (1969) [Sov. Phys.—JETP **30**, 362 (1970)].

[21]J. R. Barker, J. Phys. C **6**, 2663 (1973).

[22]D. C. Langreth, in *Linear and Non-linear Electron Transport in Solids,* edited by J. T. Devreese and E. van Boren (Plenum, New York, 1976); D. C. Langreth and J. W. Wilkins, Phys. Rev. B **6**, 3189 (1972).

[23]A. P. Jauho and J. W. Wilkins, Phys. Rev. B **29**, 1919 (1984).

[24]A. Blandin, A. Nourtier, and D. W. Hone, J. Phys. (Paris) **37**, 369 (1976).

[25]P. Danielewicz, Ann. Phys. (N.Y.) **152**, 239 (1984).

[26]D. Calecki and N. Pottier, J. Phys. (Paris) Colloq. **42**, C7-271 (1981).

[27]Sanjoy K. Sarker, Phys. Rev. B **32**, 743 (1985).

[28]D. C. Langreth, Phys. Rev. **148**, 707 (1966).

[29]Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions,* (National Bureau of Standards, Washington, D.C., 1970).

[30]G. D. Mahan and W. Hänsch, J. Phys. F **13**, L47 (1983); W. Hänsch and G. D. Mahan, Phys. Rev. B **28**, 1902 (1983).

[31]E. G. S. Paige, in *Progress in Semiconductors,* edited by A. F. Gibson and R. E. Burgess (Heywood, Temple Press, London, 1964), Vol. 8.

[32]J. E. G. Farina, in *The International Encyclopaedia of Physical Chemistry and Chemical Physics,* edited by R. McWeeny (Pergamon, Oxford, 1983), Vol. 4.

[33]G. Rickayzen, *Green's Functions and Condensed Matter* (Academic, London, 1980).

[34]J. M. Ziman, *Elements of Advanced Quantum Theory* (Cambridge University Press, Cambridge, 1969).

[35]Y. C. Chang, D. Z.-Y. Ting, J. Y. Tang, and K. Hess, Appl. Phys. Lett. **42**, 76 (1983); Lino Reggiani, Paolo Lugli, and A.-P. Jauho (unpublished).

[36]O. Ziep and R. Keiper, Phys. Status Solidi. B **128**, 779 (1985); R. Keiper and O. Ziep, *ibid.* **131**, K91-6 (1985).